Supporting Information

Metal-Free Direct 1,6- and 1,2-Difunctionalization Triggered by Radical Trifluoromethylation of Alkenes

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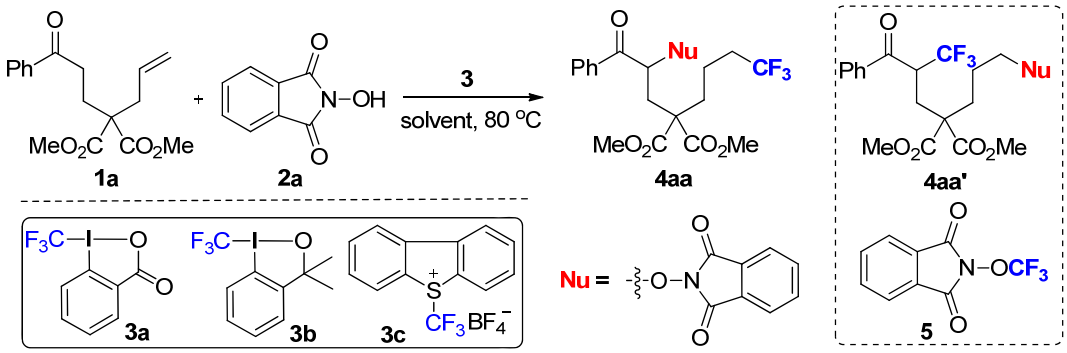
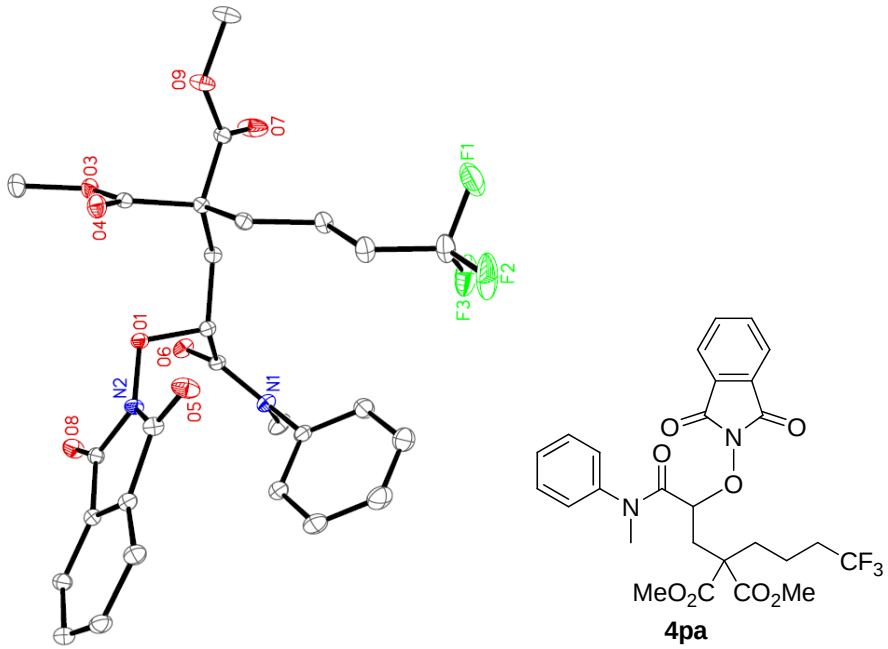
Table S1. Optimization of the Reaction Conditions[a]



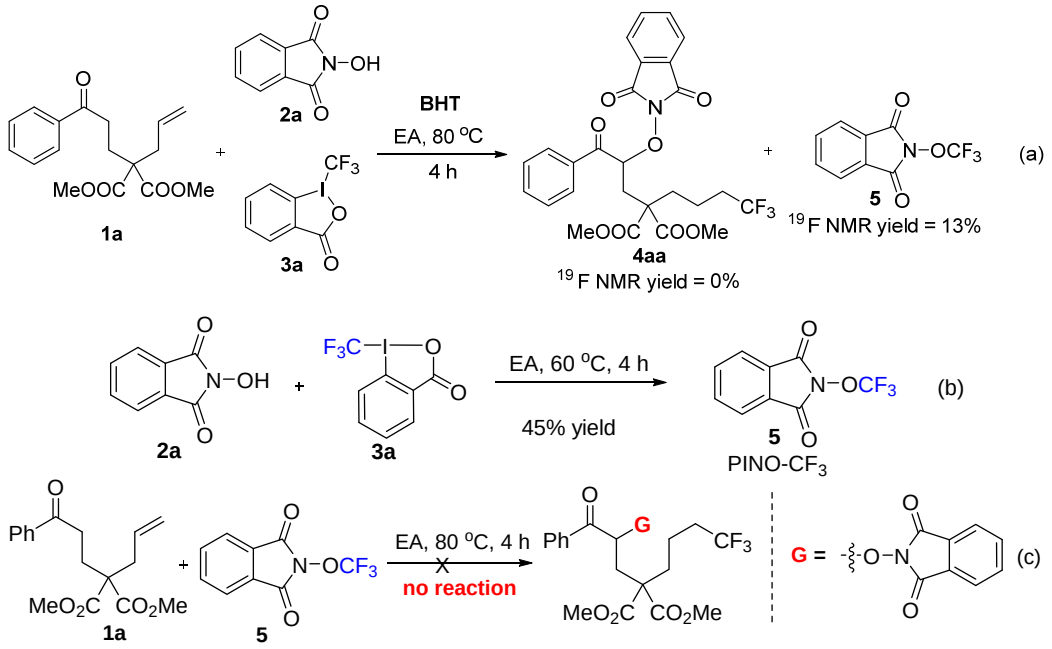
entry	solvent	**2a** (x eq.)	**3a** (y eq.)	yield (%)[b]
1	THF	2	2	25
2	DCE	2	2	67
3	CH_3CN	2	2	86
4	dioxane	2	2	69
5	EA	2	2	90
6	*i*-propyl acetate	2	2	56
7[c]	EA	2	2	72
8[d]	EA	2	2	--[e]
9	EA	1.8	1.8	82
10	EA	1.6	1.6	75
11	EA	1.5	2.0	79
12[f]	EA	2	2	88

[a] Reaction conditions: (Unless otherwise mentioned) **1a** (0.1 mmol), **2a**, and **3a** in dry solvents at 80 °C for 4 hours under argon. [b] Determined by ^{19}F NMR spectroscopy using $PhCF_3$ as an internal standard. [c] Togni's reagent **2b** was used. [d] Umemoto's reagent **2c** was used. [e] Product was not detected. [f] The reaction was conducted in the dark.

Figure S1. X-ray structure of **4pa**. All hydrogen is omitted clarity.



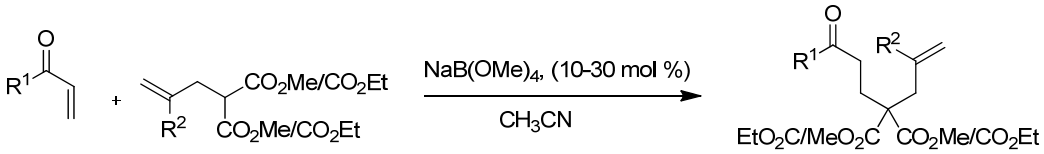
Scheme S1. Experiments for Mechanistic Study.



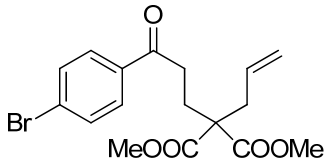
General information

All reactions were carried out under argon (Ar) atmosphere using Schlenk techniques with magnetic stirring. Reagents were purchased at the highest commercial quality and used without further purification, unless otherwise stated. Ethyl acetate (EA) was purchased anhydrous from commercial sources and transferred under an argon atmosphere. Analytical thin layer chromatography (TLC) was performed on precoated silica gel 60 F254 plates. Flash column chromatography was performed using Tsingdao silica gel (60, particle size 0.040-0.063 mm). Visualization on TLC was achieved by use of UV light (254 nm) or iodine. NMR spectra were recorded on a Bruker DPX 400 spectrometer at 400 MHz for ^{1}H NMR, 100 MHz for ^{13}C NMR and 376 MHz for ^{19}F NMR in $CDCl_3$ with tetramethylsilane (TMS) as internal standard. Chemical shifts are reported in ppm and coupling constants are given in Hz. Data for ^{1}H NMR are recorded as follows: chemical shift (ppm), multiplicity (s, singlet; d, doublet; t, triplet; q, quarter; m, multiplet), coupling constant (Hz), integration. Data for ^{13}C NMR are reported in terms of chemical shift (δ, ppm). ^{19}F NMR spectra were recorded on a Bruker DPX 400 MHz spectrometer [$CFCl_3$ as an external reference (0 ppm)]. HMRS were obtained on a Bruker Apex IV RTMS.

Typical experimental procedures for the synthesis of substrates [2, 3]



To a solution of Michael donor (1.0 mmol) and $NaB(OMe)_4$ (0.10-0.30 mmol, 10-30 mol %) in MeCN (3 mL) was added *α,β*-unsaturated ketone (1.0-2.0 mmol) at room temperature. The resulting solution was stirred at room temperature or 50 ^{o}C under air atmosphere and monitored by TLC. Upon completion, solvent was removed under reduced pressure, and the residue was purified by flash column chromatography on silica gel (ethyl acetate/petroleum ether = 1/12-1/4) to give the desired products in good yield. (Substrates **1a**, **1d**, **1e**, **1j**, **1l, 1r, 1s** were synthesized according to the reported procedure. [3, 4, 5])



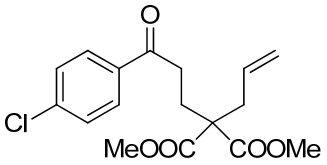
1b

Dimethyl 2-allyl-2-(3-(4-bromophenyl)-3-oxopropyl) malonate (1b)

White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, J = 8.8 Hz, 2H), 7.60 (d, J = 8.8 Hz, 2H), 5.74-5.63 (m, 1H), 5.16-5.10 (m, 1H), 3.72 (s, 6H), 2.98 (t, J = 8.0 Hz, 2H), 2.71 (d, J = 8.0 Hz, 2H), 2.30 (t, J = 8.0 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 197.8, 171.4, 135.3, 132.1, 131.9, 129.6, 128.3, 119.5, 57.0, 52.6, 38.6, 33.8, 27.3.

HRMS (ESI) calcd. for $C_{17}H_{19}BrO_5Na$ [M+Na] 405.0308, found 405.0309.



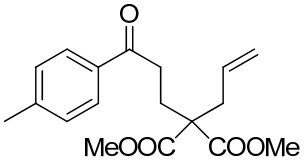
1c

Dimethyl 2-allyl-2-(3-(4-chlorophenyl)-3-oxopropyl) malonate (1c)

White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, J = 8.4 Hz, 2H), 7.42 (d, J = 8.4 Hz, 2H), 5.74-5.63 (m, 1H), 5.16-5.10 (m, 2H), 3.72 (s, 6H), 2.98 (t, J = 7.6 Hz, 2H), 2.70 (d, J = 7.0 Hz, 2H), 2.30 (t, J = 7.6 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 197.6, 171.4, 139.6, 135.0, 132.1, 129.5, 128.9, 119.4, 56.98, 52.5, 38.6, 33.8, 27.4.

HRMS (ESI) calcd. for $C_{17}H_{19}ClO_5Na$ [M+Na] 361.0813, found 361.0815.



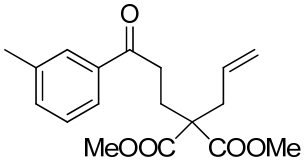
1f

Dimethyl 2-allyl-2-(3-oxo-3-(*p*-tolyl)propyl) malonate (1f)

White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, J = 8.0 Hz, 2H), 7.25 (d, J = 8.0 Hz, 2H), 5.75-5.65 (m, 1H), 5.16-5.05 (m, 2H), 3.72 (s, 6H), 2.98 (t, J = 7.6 Hz, 2H), 2.71 (d, J = 7.6 Hz, 2H), 2.41 (s, 3H), 2.32 (t, J = 8.0 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 198.6, 171.6, 144.0, 134.4, 132.3, 129.4, 128.3, 119.5, 57.2, 52.6, 38.6, 33.7, 27.5, 21.8.

HRMS (ESI) calcd. for $C_{18}H_{22}O_5Na$ [M+Na] 341.1359, found 341.1359.



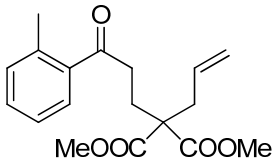
1g

Dimethyl 2-allyl-2-(3-oxo-3-(*m*-tolyl)propyl) malonate (1g)

White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76-7.74 (m, 2H), 7.39-7.32 (m, 2H), 5.76-5.65(m, 1H), 5.17-5.10 (m, 2H), 3.73 (s, 6H), 2.99 (t, J = 8.0 Hz, 2H), 2.72 (d, J = 7.2 Hz, 2H), 2.41 (s, 3H), 2.32 (t, J = 8.0 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 199.0, 171.4, 138.4, 136.7, 133.9, 132.2, 128.5, 128.5, 125.3, 119.4, 57.1, 52.5, 38.4, 33.7, 27.3, 21.4.

HRMS (ESI) calcd. for $C_{18}H_{22}O_5Na$ [M+Na] 341.1359, found 341.1358.



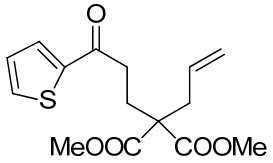
1h

Dimethyl 2-allyl-2-(3-oxo-3-(*o*-tolyl)propyl) malonate (1h)

White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.0 Hz, 1H), 7.32 (td, *J* = 7.6, 1.6 Hz, 1H), 7.26-7.21 (m, 2H), 5.75-5.64 (m, 1H), 5.16-5.09 (m, 2H), 3.72 (s, 6H), 2.93 (t, *J* = 8.0 Hz, 1H), 2.70 (d, *J* = 7.6 Hz, 2H), 2.48 (s, 3H), 2.30 (t, *J* = 8.0 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 202.5, 171.3, 138.1, 137.5, 132.2, 131.9, 131.3, 128.5, 125.7, 119.3, 56.9, 52.4, 38.3, 36.4, 27.2, 21.3.

HRMS (ESI) calcd. for $C_{18}H_{22}O_5Na$ [M+Na] 341.1359, found 341.1360.



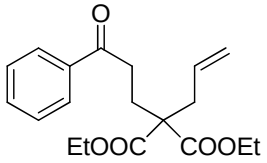
1i

Dimethyl 2-allyl-2-(3-oxo-3-(thiophen-2-yl)propyl) malonate (1i)

Pale yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.63 (dd, *J* = 4.8, 1.2 Hz, 1H), 7.13 (dd, *J* = 5.2, 3.6 Hz, 1H), 5.74-5.64 (m, 1H), 5.16-5.10 (m, 2H), 3.73 (s, 6H), 2.94 (t, *J* = 8.0 Hz, 2H), 2.70 (d, *J* = 7.2 Hz, 2H), 2.32 (t, *J* = 8.0 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 191.9, 171.4, 144.0, 133.7, 132.2, 132.1, 128.2, 119.6, 57.2, 52.6, 38.5, 34.7, 27.8.

HRMS (ESI) calcd. for $C_{15}H_{19}O_5S$ [M+H] 311.0948, found 311.0948.



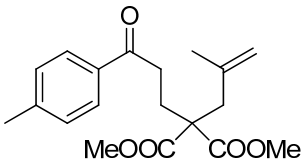
1k

Diethyl 2-allyl-2-(3-oxo-3-phenylpropyl) malonate (1k)

White solid . ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.0 Hz, 2H), 7.56 (d, *J* = 7.6 Hz, 1H), 7.45 (d, *J* = 8.0 Hz, 2H), 5.76-5.66 (m, 1H), 5.17-5.10 (m, 2H), 4.30-4.11 (m, 4H), 3.02 (t, *J* = 8.0 Hz, 2H), 2.72 (d, *J* = 7.6 Hz, 2H), 2.32 (t, *J* = 8.0 Hz, 2H), 1.25 (t, *J* = 7.2 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 199.0, 171.1, 136.8, 133.2, 132.4, 128.7, 128.2, 119.4, 61.50, 56.9, 38.4, 33.9, 27.3, 14.2.

HRMS (ESI) calcd. for $C_{19}H_{24}O_5Na$ [M+Na] 355.1516, found 355.1516.



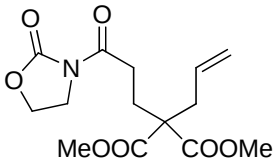
1m

Dimethyl 2-(2-methylallyl)-2-(3-oxo-3-(*p*-tolyl)propyl) malonate (1m)

White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.4 Hz, 2H), 7.25 (d, *J* = 7.6 Hz, 2H), 4.88 (t, *J* = 1.6 Hz, 1H), 4.77 (s, 1H), 3.72 (s, 6H), 2.96 (d, *J* = 8.0 Hz, 2H), 2.79 (s, 2H), 2.40 (s, 3H), 2.33 (dd, *J* = 8.0, 7.6 Hz, 2H), 1.67 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 198.4, 171.8, 143.9, 140.3, 134.2, 129.3, 128.2, 116.0, 56.51, 52.5, 41.7, 33.8, 27.4, 23.1, 21.6.

HRMS (ESI) calcd. for $C_{19}H_{24}O_5Na$ [M+Na] 355.1516, found 355.1516.



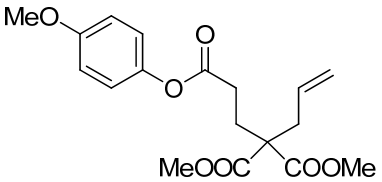
1n

Dimethyl 2-allyl-2-(3-oxo-3-(2-oxooxazolidin-3-yl)propyl) malonate (1n)

White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.54-5.44 (m, 1H), 4.98-4.91 (m, 2H), 4.27 (t, *J* = 8.0 Hz, 2H), 3.84 (t, *J* = 8.0 Hz, 2H), 3.54 (s, 6H), 2.73 (t, *J* = 8.0 Hz, 2H), 2.48 (d, *J* = 7.6 Hz, 2H), 2.03 (t, *J* = 8.0 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.5, 171.4, 153.5, 132.2, 119.6, 62.19, 57.0, 52.7, 42.7, 37.8, 30.5, 27.4.

HRMS (ESI) calcd. for $C_{14}H_{19}NO_7Na$ [M+Na] 336.1054, found 336.1055.



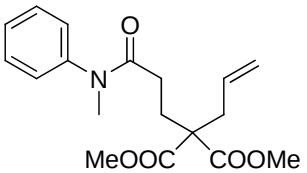
1o

1-(4-methoxyphenyl) 3,3-Dimethyl hex-5-ene-1,3,3-tricarboxylate (1o)

Colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.99 (dd, *J* = 6.8, 2.4 Hz, 2H), 6.87 (dd, *J* = 6.8, 2.4 Hz, 2H), 5.74-5.63 (m, 1H), 5.17-5.12 (m, 2H), 3.80 (s, 3H), 3.74 (s, 6H), 2.67 (d, *J* = 7.2 Hz, 2H), 2.58 (t, *J* = 7.6 Hz, 2H), 2.32 (t, *J* = 7.6 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.5, 171.2, 157.2, 144.1, 131.9, 122.2, 119.6, 114.4, 56.9, 55.5, 52.6, 38.0, 29.6, 27.8.

HRMS (ESI) calcd. for $C_{18}H_{22}O_7Na$ [M+Na] 373.1258, found 373.1257.



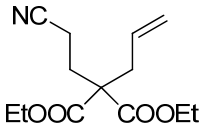
1p

Dimethyl 2-allyl-2-(3-(methyl(phenyl)amino)-3-oxopropyl) malonate (1p)

Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 (t, *J* = 7.6 Hz, 2H), 7.11 (t, *J* = 7.6Hz, 1H), 6.96 (d, *J* = 7.6 Hz, 2H), 5.33-5.27 (m, 1H), 4.77-4.68 (m, 2H), 3.34 (s, 6H), 2.99 (s, 3H), 2.24 (d, *J* = 7.6 Hz, 2H), 1.97-1.93 (m, 2H), 1.81 (t, *J* = 7.6 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 171.4, 170.8, 143.7, 131.8, 129.6, 127.6, 127.1, 118.8, 56.6, 52.0, 37.2, 37.0, 28.8, 28.3.

HRMS (ESI) calcd. for $C_{18}H_{24}NO_5$ [M+H] 334.1649, found 334.1650.



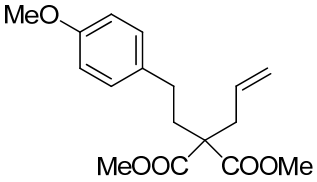
1q

Dimethyl 2-allyl-2-(2-cyanoethyl) malonate (1q)

Colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.68-5.58 (m,1H), 5.19-5.19 (m, 2H), 4.25-4.19 (m, 4H), 2.66 (d, *J* = 6.8 Hz, 2H), 2.44 (t, *J* = 7.6 Hz, 2H), 2.22 (t, *J* = 7.2 Hz, 2H), 1.30-1.25 (m, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 170.1, 131.5, 120.2, 119.2, 62.0, 56.3, 38.0, 28.9, 14.2, 13.0.

HRMS (ESI) calcd. for $C_{13}H_{19}NO_4Na$ [M+Na] 276.1206, found 276.1205.



1r

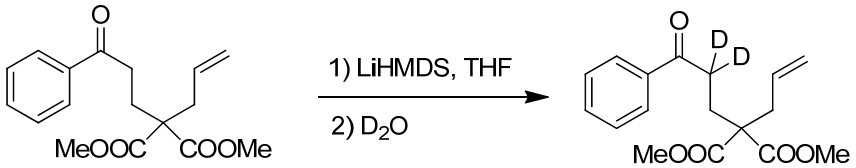
Dimethyl 2-allyl-2-(4-methoxyphenethyl)malonate (1r)

Colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.08 (d, *J* = 8.8 Hz, 2H), 6.82 (d, *J* = 8.8 Hz, 2H), 5.71-5.62 (m, 1H), 5.17-5.10 (m, 2H), 3.77 (s, 3H), 3.72 (s, 6H), 2.74 (d, *J* = 7.6 Hz, 2H), 2.49-2.45 (m, 2H), 2.18-2.13 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 171.6, 158.0, 133.3, 132.4, 129.3, 119.1, 113.8, 57.5, 55.2, 52.4, 37.4, 34.6, 29.6.

HRMS (ESI) calcd. for $C_{17}H_{23}O_5H$ [M+H] 307.1540, found 307.1541.

Experimental procedures for the synthesis of [D_2]-1a



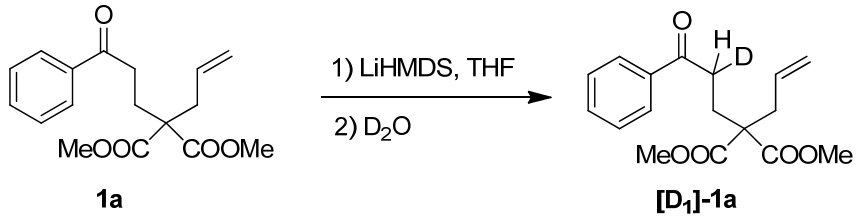
1a **[D_2]-1a**

Dimethyl 2-allyl-2-(3-(4-bromophenyl)-3-oxopropyl) malonate-*d*$_2$ ([D_2]-1a).

To a solution of **1a** (608.0 mg, 2.0 mmol) in THF (3.0 mL) at -78 °C was slowly added a solution of LiHMDS (5.0 mL, 1.0 M in THF) under argon. After being stirred

for 1 h at -78 °C, the reaction mixture was quenched by slowly sequential addition of D_2O (2.0 mL). Then the mixture was warmed to room temperature, stirred for an additional 30 min, and extracted with ethyl acetate (3 x 5.0 mL). The combined organic extracts were washed with brine (5.0 mL), dried over Na_2SO_4, filtered, and concentrated. The residue was repeated three times as the procedure described above and purified by flash chromatography on silica gel (ethyl acetate/petroleum ether = 1/12-1/6) to give the dimethyl 2-allyl-2-(3-(4-bromophenyl)-3-oxopropyl) malonate-*d₂* (**[D₂]-1a**) (535.0 mg, 88% yield) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97-7.94 (m, 2H), 7.61-7.52 (m, 1H), 7.48-7.44 (m, 2H), 5.73-5.65 (m, 7.3 Hz, 1H), 5.17-5.10 (m, 2H), 3.73 (s, 6H), 3.01-2.97 (m, 0.16H), 2.72 (d, *J* = 7.2 Hz, 2H), 2.31 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.9, 171.4, 136.6, 133.1, 132.1, 128.6, 128.0, 119.4, 57.0, 52.5, 38.4, 32.9, 27.2. HRMS (ESI) calcd. for $C_{17}H_{18}D_2O_5Na$ [M+Na] 329.1328, found 329.1325.

Synthetic procedure for [D₁]-1a



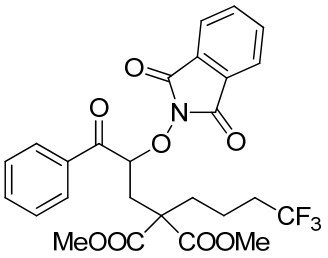
Dimethyl 2-allyl-2-(3-(4-bromophenyl)-3-oxopropyl) malonate-*d₁* ([D₁]-1a)

To a solution of **1a** (608.0 mg, 2.0 mmol) in THF (3.0 mL) at -78 °C was slowly added a solution of LiHMDS (2.0 ml, 1.0 M in THF) under argon. After being stirred for 1 h at -78 °C, the reaction mixture was quenched by slowly sequential addition of D_2O (2.0 mL). The mixture was warmed to room temperature, stirred for an additional 30 min, and extracted with ethyl acetate (3 x 5.0 mL). The combined organic extracts were washed with brine (5.0 mL), dried over Na_2SO_4, filtered, and concentrated. The residue was purified by flash chromatography on silica gel (ethyl acetate/petroleum ether = 1/12-1/6) to give the dimethyl 2-allyl-2-(3-(4-bromophenyl)-3-oxopropyl) malonate-*d₁* (**[D₁]-1a**) (585.0 mg, 96% yield) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96-7.94 (m, 2H), 7.58-7.54 (m, 1H), 7.48-7.44 (m, 2H), 5.75-5.65 (m, 1H), 5.17-5.10 (m, 2H), 3.73 (s, 6H), 3.08-2.90 (m, 0.93H), 2.72 (d, *J* = 7.2 Hz, 2H), 2.32 (d, *J* = 7.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.8, 171.4, 136.6, 133.1, 132.1, 128.6, 128.0, 119.4, 57.0, 52.5, 38.4, 33.4, 27.2. HRMS (ESI) calcd. for $C_{17}H_{19}DO_5Na$ [M+Na] 328.1266, found 328.1266.

General procedure for trifluoromethylation of alkenes toward trifluoromethyl *α*-hydroxycarbonyl or *α*-hydroxytrifluoromethyl compounds

To a flame-dried Schlenk tube equipped with a magnetic stir bar were added **1** (0.5 mmol), Togni's reagent **3a** (316.0 mg, 1.0 mmol) and **2a (NHPI)** or **2b (HOBT)** or **2c (NHBO)** (1.0 mmol). The tube was evacuated and backfilled with argon for three times, and ethyl acetate (5.0 mL) was added *via* syringe. The tube was stirred at 60-80 °C and monitored by TLC. After completion, solvent was removed under

reduced pressure, and the residue was purified by flash column chromatography on silica gel (ethyl acetate/petroleum ether = 1/8-1/2) to give the corresponding products.



4aa

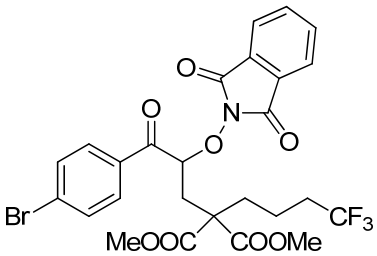
Dimethyl 2-(2-((1,3-dioxoisoindolin-2-yl)oxy)-3-oxo-3-phenylpropyl)-2-(4,4,4-trifluorobutyl) malonate (4aa)

White solid (90% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, J = 7.2 Hz, 2H), 7.72-7.70 (m, 2H), 7.66-7.64 (m, 2H), 7.54-7.49 (m, 1H), 7.43-7.39 (m, 2H), 5.81 (dd, J = 5.6, 3.2 Hz, 1H), 3.60 (s, 3H), 3.47 (s, 3H), 2.73 (dd, J = 15.2, 5.6 Hz, 1H), 2.56 (dd, J = 15.2, 5.2 Hz, 1H), 2.21-1.99 (m, 4H), 1.53-1.37 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 193.7, 170.9, 170.6, 163.4, 134.7, 134.6，134.0, 129.3, 128.8, 128.6, 126.8 (q, J_{CF} = 274.0 Hz), 123.7, 83.0, 55.9, 52.9, 52.6, 33.7 (q, J_{CF} = 29.0 Hz), 33.0, 32.9, 17.3 (q, J_{CF} = 3.0 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -66.3 (t, J = 11.3 Hz, 3F).

HRMS (ESI) calcd. for $C_{26}H_{24}F_3NO_8Na$ [M+Na] 558.1346, found 558.1346.



4ba

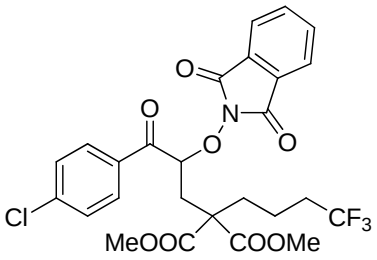
Dimethyl 2-(3-(4-bromophenyl)-2-((1,3-dioxoisoindolin-2-yl)oxy)-3-oxopropyl)-2-(4,4,4-trifluorobutyl) malonate (4ba)

White solid (79% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, J = 8.4 Hz, 2H), 7.84-7.80 (m, 2H), 7.81-7.75 (m, 2H), 7.66 (d, J = 8.4 Hz, 2H), 5.74 (t, J = 5.6 Hz, 1H), 3.69 (s, 3H), 3.56 (s, 3H), 2.77 (dd, J = 15.2, 6.4 Hz, 1H), 2.58 (dd, J = 15.2, 5.2 Hz, 1H), 2.21-2.10 (m, 4H), 1.63-1.46 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 192.7, 170.9, 170.5, 163.5, 134.81, 133.3, 132.1, 131.0, 129.4, 128.6, 126.8 (q, J_{CF} = 275.0 Hz), 123.7, 83.4, 55.8, 52.9, 52.7, 33.7 (q, J_{CF} = 28.0 Hz), 33.1, 32.9, 17.3 (q, J_{CF} = 3.0 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -66.3 (s, 3F).

HRMS (ESI) calcd. for $C_{26}H_{23}BrF_3NO_8Na$ [M+Na] 636.0451, found 636.0454.



4ca

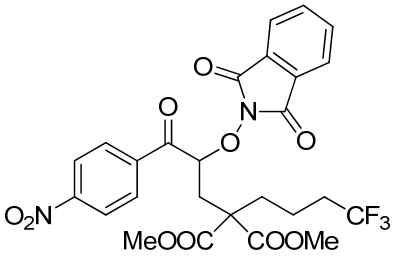
Dimethyl 2-(3-(4-chlorophenyl)-2-((1,3-dioxoisoindolin-2-yl)oxy)-3-oxopropyl)-2-(4,4,4-trifluorobutyl) malonate (4ca)

White solid (70% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, *J* = 8.8, 2H), 7.83-7.81 (m, 2H), 7.78-7.75 (m, 2H), 7.49 (d, *J* = 6.8, Hz, 2H), 5.76 (t, *J* = 5.2, Hz ,1H), 3.69 (s, 3H), 3.56 (s, 3H), 2.80 (dd, *J* = 15.2, 6.4 Hz, 1H), 2.61 (dd, *J* = 15.2, 5.2 Hz, 1H), 2.21-2.07 (m, 4H), 1.61-1.47 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 192.6, 171.0, 170.7, 163.6, 140.6, 134.9, 133.1, 131.0, 129.2, 128.8, 126.9 (q, J_{CF} = 275.0 Hz), 123.8, 83.6, 56.0, 53.0, 52.8, 33.8 (q, J_{CF} = 29.0 Hz), 33.2, 33.0, 17.4 (q, J_{CF} = 3.0 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -66.3 (s, 3F).

HRMS (ESI) calcd. for $C_{26}H_{24}ClF_3NO_8$ [M+H] 570.1137, found 570.1137.



4da

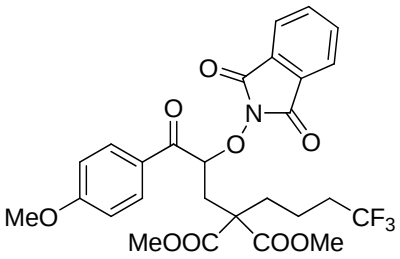
Dimethyl 2-(2-((1,3-dioxoisoindolin-2-yl)oxy)-3-(4-nitrophenyl)-3-oxopropyl)-2-(4,4,4-trifluorobutyl) malonate (4da)

White solid (61% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (d, *J* = 8.8, Hz, 2H), 8.37 (d, *J* = 8.8, Hz, 2H), 7.85-7.82 (m, 2H), 7.80-7.77 (m, 2H), 5.75 (dd, *J* = 6.8, 4.4 Hz, 1H), 3.69 (s, 3H), 3.58 (s, 3H), 2.84 (dd, *J* = 15.2, 6.8 Hz, 1H), 2.63 (dd, *J* = 15.2, 4.0 Hz, 1H), 2.19-2.08 (m, 4H), 1.61-1.50 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 192.3, 170.9, 170.6, 163.5, 150.6, 139.2, 134.9, 130.7, 128.5, 126.8 (q, J_{CF} = 275.0 Hz), 123.8, 123.8, 84.0, 55.9, 52.9, 52.8, 33.7 (q, J_{CF} = 29.0 Hz), 33.2, 32.7, 17.3 (q, J_{CF} = 3.0 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -66.2. (s, 3F).

HRMS (ESI) calcd. for $C_{26}H_{23}F_3N_2O_{10}Na$ [M+Na] 603.1197, found 603.1194.



4ea

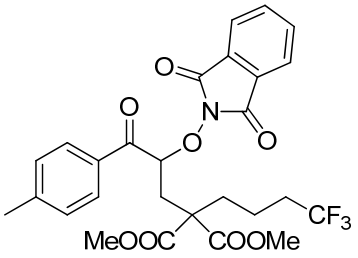
Dimethyl 2-(2-((1,3-dioxoisoindolin-2-yl)oxy)-3-(4-methoxyphenyl)-3-oxopropyl) -2-(4,4,4-trifluorobutyl) malonate (4ea)

White solid (83% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, J = 8.8 Hz, 2H), 7.82-7.79(m, 2H), 7.76-7.72 (m, 2H), 6.97 (d, J = 8.8 Hz, 2H), 5.84 (t, J = 5.6 Hz, 1H), 3.87 (s, 3H), 3.69 (s, 3H), 3.57 (s, 3H), 2.80 (dd, J = 15.6, 6.0 Hz, 1H), 2.64 (dd, J = 15.6, 5.6 Hz, 1H), 2.24-2.05 (m, 4H), 1.59-1.47 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 192.0, 171.0, 170.6, 164.2, 163.4, 134.7, 131.8, 128.7, 127.7, 126.8 (q, J_{CF} = 275.0 Hz), 123.6, 114.0, 83.0, 55.9, 55.5, 52.8, 52.6, 33.7 (q, J_{CF} = 29.0 Hz), 33.1, 32.9, 17.3 (q, J_{CF} = 3.0 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -66.3 (s, 3F).

HRMS (ESI) calcd. for $C_{27}H_{27}F_3NO_9$ [M+H] 598.1632, found 598.1633.



4fa

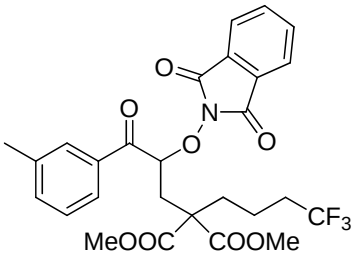
Dimethyl 2-(2-((1,3-dioxoisoindolin-2-yl)oxy)-3-oxo-3-(*p*-tolyl)propyl)-2-(4,4,4-tri fluorobutyl) malonate (4fa)

White solid (83% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, J = 8.4 Hz, 2H), 7.81-7.78 (m, 2H), 7.75-7.72 (m, 2H), 7.30 (d, J = 8.0 Hz, 2H), 5.87 (t, J = 5.6, Hz, 1H), 3.70 (s, 3H), 3.58 (s, 3H), 2.79 (dd, J = 15.2, 5.6 Hz, 1H), 2.64 (dd, J = 15.2, 5.6 Hz, 1H), 2.41 (s, 3H), 2.28-2.05 (m, 4H), 1.63-1.47 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 193.4, 171.0, 170.6, 163.4, 145.1, 134.7, 132.1, 129.5, 129.4, 126.8 (q, J_{CF} = 275.0 Hz), 128.7, 123.6, 83.0, 55.9, 52.9, 52.6, 33.8 (q, J_{CF} = 29.0 Hz), 33.1, 32.8, 21.7, 17.3 (q, J_{CF} = 3.0 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -66.3 (s, 3F).

HRMS (ESI) calcd. for $C_{27}H_{26}F_3NO_8Na$ [M+Na] 572.1503, found 572.1500.



4ga

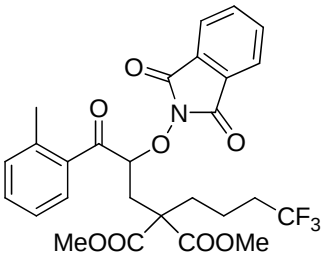
Dimethyl 2-(2-((1,3-dioxoisoindolin-2-yl)oxy)-3-oxo-3-(*m*-tolyl)propyl)-2-(4,4,4-trifluorobutyl) malonate (4ga)

White solid (65% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97-7.95 (m, 2H), 7.82-7.79 (m, 2H), 7.75-7.72 (m, 2H), 7.42-7.36 (m, 2H), 5.90 (t, J =5.6 Hz, 1H), 3.70 (s, 3H), 3.58 (s, 1H), 2.80 (dd, J = 15.2, 5.6 Hz, 1H), 2.64 (dd, J = 15.2, 5.6 Hz, 1H), 2.42 (s, 3H), 2.26-2.11 (m, 4H), 1.59-1.49(m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 193.9, 171.0, 170.6, 163.4, 138.7, 134.8, 134.7, 134.7, 129.73, 128.7, 128.6, 126.4, 126.8 (q, J_{CF} = 275.0 Hz), 123.6, 83.0, 55.9, 52.9, 52.7, 33.8 (q, J_{CF} = 29.0 Hz), 33.0, 32.8, 21.3, 17.3 (q, J_{CF} = 3.0 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -66.3 (s, 3F).

HRMS (ESI) calcd. for $C_{27}H_{26}F_3NO_8Na$ [M+Na] 572.1503, found 572.1502.



4ha

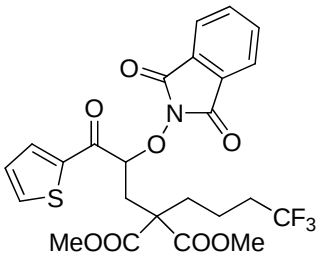
Dimethyl 2-(2-((1,3-dioxoisoindolin-2-yl)oxy)-3-oxo-3-(*o*-tolyl)propyl)-2-(4,4,4-trifluorobutyl) malonate (4ha)

White solid (81% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83-7.79 (m, 3H), 7.75-7.72 (m, 2H), 7.41-7.37 (m, 1H), 7.28 (t, J = 7.2 Hz, 2H), 5.93 (t, J =5.6 Hz, 1H), 3.65 (s, 3H), 3.63 (s, 3H), 2.62-2.61 (m, 2H), 2.50 (s, 3H), 2.30-2.24 (m, 2 H), 2.18-2.10 (m, 2 H), 1.56-1.50 (m, 1H), 1.47-1.41 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 196.8, 170.9, 170.7, 163.3, 140.0, 134.7, 132.4, 132.2, 129.1, 128.6, 126.8 (q, J_{CF} = 275.0 Hz), 125.7, 123.6, 83.4, 55.8, 52.8, 52.7, 31.7 (q, J_{CF} = 29.0 Hz), 32.7, 32.2, 21.2, 17.2 (q, J_{CF} = 3.0 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -66.3 (s, 3F).

HRMS (ESI) calcd. for $C_{27}H_{26}F_3NO_8Na$ [M+Na] 572.1503, found 572.1503.



4ia

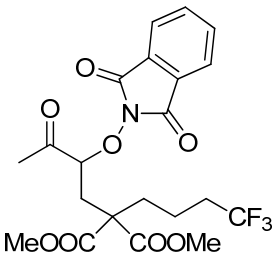
Dimethyl 2-(2-((1,3-dioxoisoindolin-2-yl)oxy)-3-oxo-3-(thiophen-2-yl)propyl)-2-(4 ,4,4-trifluorobutyl) malonate (4ia)

White solid (75% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26-8.24 (m, 1H), 7.81-7.51 (m, 5H), 7.22-7.20 (m, 1H), 5.69 (t, J = 5.6 Hz, 1H), 3.71 (s, 3H), 3.61 (s, 3H), 2.82 (dd, J = 15.6, 5.6 Hz, 1H), 2.68 (dd, J = 15.6, 5.6 Hz, 1H), 2.26-2.11 (m, 4H), 1.61-1.49 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 186.7, 170.9, 170.6, 163.4, 141.5, 135.7, 134.8, 134.7, 128.7, 128.6, 126.8 (q, J_{CF} = 275.0 Hz), 123.7, 84.2, 55.8, 52.9, 52.7, 33.8 (q, J_{CF} = 29.0 Hz), 33.3, 32.8, 17.3 (q, J_{CF} = 3.0 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -66.3 (s, 3F).

HRMS (ESI) calcd. for $C_{24}H_{22}F_3NO_8SNa$ [M+Na] 564.0910, found 564.0911.



4ja

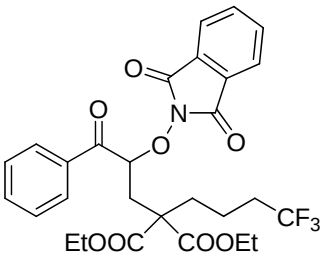
Dimethyl 2-(2-((1,3-dioxoisoindolin-2-yl)oxy)-3-oxobutyl)-2-(4,4,4-trifluorobutyl) malonate (4ja)

White solid (66% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85-7.81 (m, 2H), 7.79-7.76 (m, 2H), 4.65 (t, J = 5.6 Hz, 1H), 3.72 (s, 3H), 3.71 (s, 3H), 2.61 (dd, J = 15.6.,5.6 Hz, 1H), 2.53 (dd, J = 15.6, 5.2 Hz, 1H), 2.49 (s, 3H), 2.33-2.09 (m, 4H), 1.59-1.45 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 204.5, 170.7, 170.6, 163.3, 134.8, 128.6, 126.8 (q, J_{CF} = 275.0 Hz), 123.8, 88.0, 55.8, 52.9, 52.8, 33.7 (q, J_{CF} = 29.0 Hz), 32.7, 31.9, 25.7, 17.2 (q, J_{CF} = 3.0 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -66.3 (s, 3F).

HRMS (ESI) calcd. for $C_{21}H_{22}F_3NO_8Na$ [M+Na] 496.1190, found 496.1189.



4ka

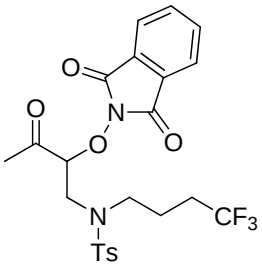
Diethyl 2-(2-((1,3-dioxoisoindolin-2-yl)oxy)-3-oxo-3-phenylpropyl)-2-(4,4,4-trifluorobutyl) malonate (4ka)

White solid (82% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (dd, *J* = 7.2, 2.8 Hz, 2H), 7.81-7.78 (m, 2H), 7.75-7.72 (m, 2H), 7.61-7.57 (m, 1H), 7.49 (d, *J* = 7.6, Hz, 2H), 5.87 (t, *J* = 5.6 Hz, 1H), 4.20-4.09 (m, 3H), 4.01-3.93 (m, 1H), 2.79 (dd, *J* = 15.2, 5.6 Hz, 1H), 2.65 (dd, *J* = 15.6, 6.0 Hz, 1H), 2.27-2.10 (m, 4H), 1.64-1.49 (m, 2H), 1.20 (t, *J* = 8.0 Hz, 3H), 1.12 (t, *J* = 8.0 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 194.1, 170.7, 170.3, 163.5, 134.8, 134.8, 134.1, 129.4, 128.9, 128.9, 127.0 (q, J_{CF} = 274.0 Hz), 123.8, 83.5, 62.0, 61.9, 56.1, 34.0 (q, J_{CF} = 29.0 Hz), 33.1, 32.8, 17.4 (q, J_{CF} = 3.0 Hz), 14.0, 13.9.

^{19}F NMR (376 MHz, $CDCl_3$) δ -66.3 (s, 3F).

HRMS (ESI) calcd. for $C_{28}H_{28}F_3NO_8Na$ [M+Na] 586.1659, found 586.1658.



4la

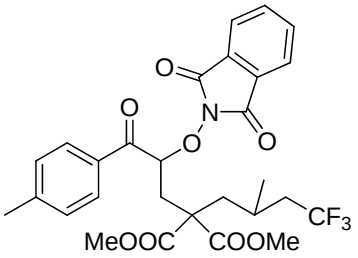
***N*-(2-((1,3-Dioxoisoindolin-2-yl)oxy)-3-oxobutyl)-4-methyl-*N*-(4,4,4-trifluorobutyl) benzenesulfonamide (4la)**

White solid (41% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86-7.82 (m, 2H), 7.80-7.77 (m, 2H), 7.68 (d, *J* = 8.4 Hz, 2H), 7.29 (d, *J* = 8.4 Hz, 2H), 4.83 (t, *J* = 5.2 Hz, 1H), 3.73 (dd, *J* = 15.6, 5.2 Hz, 1H), 3.63 (dd, *J* = 15.6, 5.6 Hz, 1H), 3.42-3.27 (m, 2H), 2.53 (s, 3H), 2.38 (s, 3H), 2.16-2.05 (m, 2H), 1.89-1.80 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 203.9, 163.2, 144.0, 135.4, 134.9, 129.9, 128.6, 127.4, 126.9 (q, J_{CF} = 275.0 Hz), 123.8, 90.7, 49.0, 48.2, 31.0 (q, J_{CF} = 29.0 Hz), 27.4, 21.5, 20.8 (q, J_{CF} = 3.0 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -66.1 (t, *J* = 11.3 Hz, 3F).

HRMS (ESI) calcd. for $C_{23}H_{24}F_3N_2O_6S$ [M+H] 513.1302, found 513.1303.



4ma

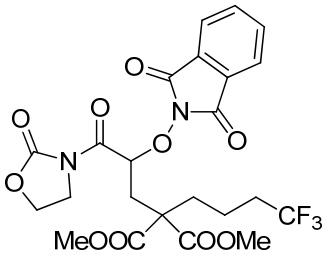
Dimethyl 2-(2-((1,3-dioxoisoindolin-2-yl)oxy)-3-oxo-3-(*p*-tolyl)propyl)-2-(4,4,4-tri fluoro-2-methylbutyl) malonate (4ma)

White solid (d:r = 1:1; 75% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (dd, J = 8.4, 6.8 Hz, 2H), 7.82-7.80 (m, 2H), 7.74-7.72 (m, 2H), 7.29 (d, J = 7.6 Hz, 2H), 5.91 (t, J = 6.0 Hz, 0.5H), 5.87 (t, J = 5.6, Hz, 0.5H), 3.68 (s, 3H), 3.53 (s, 3H), 2.86-2.75 (m, 1H), 2.70-2.57 (m, 1H), 2.41 (s, 3H), 2.27-1.96 (m, 5H), 1.00 (t, J = 6.6 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 193.1, 193.1, 171.4, 171.2, 171.0, 170.8, 163.5, 145.1, 145.1, 134.7, 132.3, 129.5(2), 129.4, 128.6, 126.8 (q, J_{CF} = 276.0 Hz), 123.6, 82.7, 82.5, 55.4, 55.1, 52.9 (q, J_{CF} = 2.0 Hz), 52.8, 52.7, 52.6 (q, J_{CF} = 2.0 Hz), 52.6, 52.5, 41.2 (q, J_{CF} = 26.0 Hz), 40.9 (q, J_{CF} = 26.0 Hz), 33.6, 33.4, 24.4, 21.7, 20.5, 20.4.

^{19}F NMR (376 MHz, $CDCl_3$) δ -63.1 (s, 3F), -63.2 (s, 3F). (**Two diastereoisomers can't be separated.**)

HRMS (ESI) calcd. for $C_{28}H_{28}F_3NO_8$ Na [M+Na] 586.1659, found 586.1659.



4na

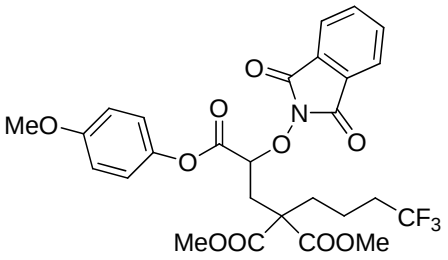
Dimethyl 2-(2-((1,3-dioxoisoindolin-2-yl)oxy)-3-oxo-3-(2-oxooxazolidin-3-yl)prop yl) -2-(4,4,4-trifluorobutyl) malonate (4na)

White solid (61% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83-7.79 (m, 2H), 7.77-7.75 (m, 2H), 6.22 (t, J = 6.0 Hz, 1H), 4.50-4.45 (m, 2H), 4.15-4.02 (m, 2H), 3.76 (s, 3H), 3.73 (s, 3H), 2.75 (d, J = 6.0 Hz, 2H), 2.33-2.15 (m, 4H), 1.65-1.53 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 171.0, 170.9, 168.7, 163.2, 153.2, 134.8, 128.6, 126.9 (q, J_{CF} = 275.0 Hz), 123.7, 79.4, 62.7, 55.8, 53.0, 52.8, 42.7, 33.7 (q, J_{CF} = 29.0 Hz), 33.3, 31.5, 17.1 (q, J_{CF} = 3.0 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -66.3 (s, 3F).

HRMS (ESI) calcd. for $C_{23}H_{23}F_3N_2O_{10}$Na [M+Na] 567.1197, found 567.1196.



4oa

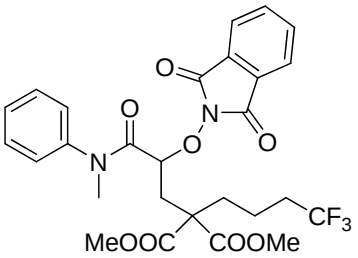
1-(4-Methoxyphenyl)3,3-dimethyl 1-((1,3-dioxoisoindolin-2-yl)oxy)-7,7,7-trifluoroheptane -1,3,3-tricarboxylate (4oa)

White solid (48% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99-7.95 (m, 2H), 7.82-7.79 (m, 2H), 7.76-7.73 (m, 2H), 7.42-7.36 (m, 2H), 5.90 (t, J = 5.6 Hz, 1H), 3.70 (s, 3H), 3.58 (s, 3H), 2.80 (dd, J = 15.6, 5.6 Hz, 1H), 2.64 (dd, J = 115.6, 5.6 Hz, 1H), 2.42 (s, 3H), 2.30-2.08 (m, 4H), 1.62-1.48 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 170.8, 170.7, 167.4, 163.0, 157.6, 143.7, 134.8, 128.7, 126.85 (q, J_{CF} = 275.0 Hz), 123.8, 122.1, 114.5, 82.2, 55.9, 55.6, 53.1, 52.9, 33.8 (q, J_{CF} = 29.0 Hz), 33.6, 31.8, 17.3 (q, J_{CF} = 3.0 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -66.3 (s, 3F).

HRMS (ESI) calcd. for $C_{27}H_{26}F_3NO_{10}Na$ [M+Na] 604.1401, found 604.1403.



4pa

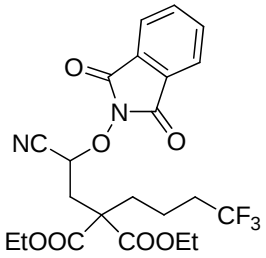
Dimethyl 2-(2-((1,3-dioxoisoindolin-2-yl)oxy)-3-(methyl(phenyl)amino)-3-oxopropyl)-2-(4,4,4-trifluorobutyl) malonate (4pa)

White solid (57% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83-7.81 (m, 2H), 7.79-7.76 (m, 2H), 7.34-7.32 (m, 3H), 7.20-7.18 (m, 2H), 4.99 (dd, J = 7.6, 5.6 Hz, 1H), 3.69 (s, 3H), 3.66 (s, 3H), 3.27 (s, 3H), 2.72 (dd, J = 15.2, 7.6 Hz, 1H), 2.56 (dd, J = 15.2, 5.6 Hz, 1H), 2.10-1.94 (m, 4H), 1.42-1.36 (m, 1H), 1.28-1.20 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.9, 170.8, 167.1, 163.2, 142.4, 134.6, 129.7, 128.8, 128.3, 127.3, 126.8 (q, J_{CF} = 275.0 Hz), 123.6, 77.8, 55.5, 52.7, 52.6, 38.0, 33.7 (q, J_{CF} = 29.0 Hz), 33.4, 31.9, 17.1 (q, J_{CF} = 3.0 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -66.1 (s, 3F).

HRMS (ESI) calcd. for $C_{27}H_{28}F_3N_2O_8$ [M+H] 565.1792, found 565.1793.



4qa

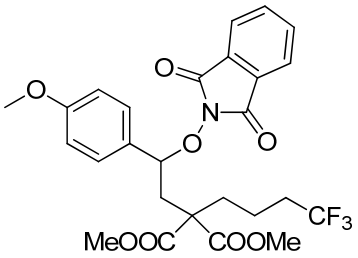
Diethyl 2-(2-cyano-2-((1,3-dioxoisoindolin-2-yl)oxy)ethyl)-2-(4,4,4-trifluorobutyl) malonate (4qa)

Colourless oil (43% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90-7.87 (m, 2H), 7.84-7.81 (m, 2H), 5.25 (t, J = 6.0 Hz, 1H), 4.29-4.24 (m, 4H), 2.83-2.72 (m, 2H), 2.24-2.15 (m, 4H), 1.61-1.53 (m, 2H), 1.31-1.23 (m, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 169.7, 169.5, 162.7, 135.1, 128.5, 126.8 (q, J_{CF} = 275.0 Hz), 124.1, 116.1, 72.0, 62.4, 62.2, 55.4, 34.9, 33.7 (q, J_{CF} = 29.0 Hz), 31.9, 17.2 (q, J_{CF} = 3.0 Hz), 13.9, 13.9.

^{19}F NMR (376 MHz, $CDCl_3$) δ -66.3 (s, 3F).

HRMS (ESI) calcd. for $C_{22}H_{24}F_3N_2O_7$ [M+H] 485.1530, found 485.1528.



4ra

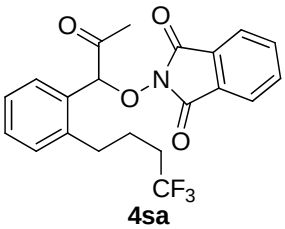
Dimethyl2-(2-((1,3-dioxoisoindolin-2-yl)oxy)-2-(4-methoxyphenyl)ethyl)-2-(4,4,4-trifluorobutyl) malonate (4ra)

White solid (59% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68-7.63 (m, 4H), 7.34 (d, J = 8.8 Hz, 2H), 6.80 (d, J = 8.4 Hz, 2H), 5.33 (dd, J = 7.6, 5.2 Hz, 1H), 3.74 (s, 3H), 3.71(s, 3H), 3.62 (s, 3H), 2.88 (dd, J = 15.2, 7.6 Hz, 1H), 2.55 (dd, J = 15.2, 5.2 Hz, 1H), 2.32-2.20 (m, 2H), 2.17-2.10 (m, 2H), 1.60-1.51 (m, 1H), 1.47-1.37 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.2, 171.0, 163.3, 160.4, 134.3, 129.7, 129.4, 128.7, 126.9 (q, J_{CF} = 275.0 Hz), 123.3, 113.7, 84.6, 55.9, 55.2, 52.7, 52.7, 37.6, 33.9 (q, J_{CF} = 29.0 Hz), 31.3, 17.2 (q, J_{CF} = 3.0 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -66.4 (s, 3F).

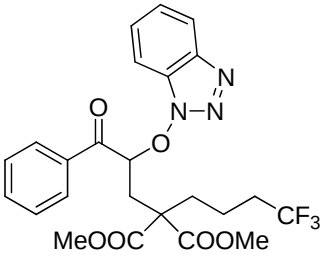
HRMS (ESI) calcd. for $C_{26}H_{26}F_3NO_8Na$ [M+Na] 560.1503, found 560.1502.



4sa

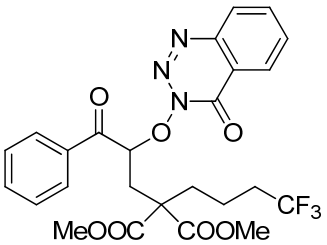
2-(2-Oxo-1-(2-(4,4,4-trifluorobutyl)phenyl)propoxy)isoindoline-1,3-dione (4sa)

White solid (84% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80-7.77 (m, 2H), 7.74-7.72 (m, 2H), 7.61-7.58 (m, 1H), 7.37-7.29 (m, 2H), 7.26-7.22 (m, 1H), 6.04 (s, 1H), 2.84 (t, J = 8.0 Hz, 2H), 2.35(s, 3H), 2.29-2.11 (m, 2H), 1.92-1.85 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 203.0, 163.3, 140.6, 134.6, 130.8, 130.0, 129.8, 129.0, 128.6, 127.0 (q, J_{CF} = 275.0 Hz), 126.9, 123.6, 89.1, 33.3 (q, J_{CF} = 28.0 Hz), 31.1, 26.3, 23.27 (q, J_{CF} = 3.0 Hz).
^{19}F NMR (376 MHz, $CDCl_3$) δ -66.2 (s, 3F).
HRMS (ESI) calcd. for $C_{21}H_{19}F_3NO_4Na$ [M+H] 406.1261, found 406.1261.



4ab

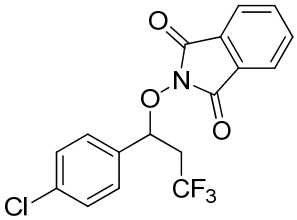
Dimethyl 2-(2-((3a,7a-dihydro-1H-benzo[d][1,2,3]triazol-1-yl)oxy)-3-oxo-3-phenylpro pyl)-2-(4,4,4-trifluorobutyl) malonate (4ab)
Yellow oil (65% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96-7.90 (m, 3H), 7.83 (d, J = 8.4 Hz 1H), 7.60-7.56 (m, 1H), 7.53-7.43 (m, 3H), 7.35-7.31 (m, 1H), 6.52 (dd, J = 8.8, 3.2 Hz, 1H), 3.77 (s, 3H), 3.74 (s, 3H), 2.74 (dd, J = 16.0, 3.2 Hz, 1H), 2.61 (dd, J = 16.0, 8.8 Hz, 1H), 2.34-2.28 (m, 2H), 2.18-2.10 (m, 2H), 1.66-1.58 (m, 1H), 1.50-1.42 (m, 1H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 194.6, 170.9, 170.8, 143.2, 134.5, 133.9, 129.0, 128.7, 128.3, 127.9, 126.7 (q, J_{CF} = 275.0 Hz), 124.8, 119.8, 110.3, 85.3, 55.9, 53.2, 53.0, 34.3, 33.8 (q, J_{CF} = 29.0 Hz), 33.1, 17.3 (q, J_{CF} = 3.0 Hz).
^{19}F NMR (376 MHz, $CDCl_3$) δ -66.3 (s, 3F).
HRMS (ESI) calcd. for $C_{24}H_{24}F_3N_3O_6Na$ [M+Na] 530.1509, found 530.1508



4ac

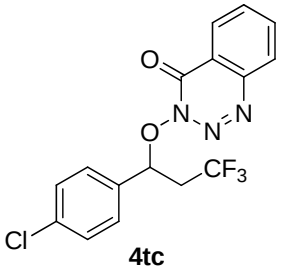
Dimethyl 2-(3-oxo-2-((4-oxobenzo[d][1,2,3]triazin-3(4H)-yl)oxy)-3-phenylpropyl) -2-(4, 4,4-trifluorobutyl) malonate (4ac)
Yellow oil (67% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, J = 8.0 Hz, 1H), 8.26-8.18 (m, 2H), 8.15 (d, J = 8.0 Hz, 1H), 7.98-7.94 (m, 1H), 7.83-7.78 (m, 1H), 7.60 (t, J = 7.8 Hz, 1H), 7.50 (t, J = 8.0 Hz, 2H), 6.08 (t, J = 5.6 Hz, 1H), 3.68 (s, 3H), 3.60 (s, 3H), 2.88 (dd, J = 15.2, 5.6 Hz, 1H), 2.78 (dd, J = 15.2, 5.6 Hz, 1H), 2.33-2.05 (m, 4H), 1.63-1.48 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 193.6, 170.9, 170.6, 151.0, 143.9, 135.2, 134.6, 134.0, 132.5, 129.4, 128.8, 126.8 (q, J_{CF} = 275.0 Hz), 125.6, 122.1, 83.9, 56.0, 52.9, 52.7, 33.7 (q, J_{CF} = 29.0 Hz), 32.9, 32.8, 17.3 (q, J_{CF} = 3.0 Hz).
^{19}F NMR (376 MHz, $CDCl_3$) δ -66.3 (s, 3F).
HRMS (ESI) calcd. for $C_{25}H_{24}F_3N_3O_7Na$ [M+Na] 558.1459, found 558.1457.



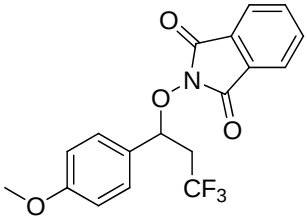
4ta

2-(1-(4-Chlorophenyl)-3,3,3-trifluoropropoxy) isoindoline-1,3-dione (4ta)
White solid (67% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76-7.70 (m, 4H), 7.45 (d, J = 8.8 Hz, 2H), 7.33 (d, J = 8.4 Hz, 2H), 5.65 (t, J = 6.4 Hz, 1H), 3.14-3.01 (m, 1H), 2.80-2.66 (m, 1H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 163.3, 135.8, 134.6, 134.4, 129.4, 128.9, 128.5, 124.8 (q, J_{CF} = 275.0 Hz), 123.6, 81.7 (q, J_{CF} = 3.0 Hz), 39.4 (q, J_{CF} = 29.0 Hz).
^{19}F NMR (376 MHz, $CDCl_3$) δ -63.2 (s, 3F).
HRMS (ESI) calcd. for $C_{17}H_{11}ClF_3NO_3Na$ [M+Na] 392.0272, found 392.0270.



4tc

3-(1-(4-Chlorophenyl)-3,3,3-trifluoropropoxy)benzo[d][1,2,3]triazin-4(3H)-one (4tc)
Yellow oil (48% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, J = 8.0, Hz, 1H), 8.12 (d, J = 8.4 Hz, 1H), 7.97-7.93 (m, 1H), 7.81-7.77 (m, 1H), 7.43 (d, J = 8.8 Hz, 2H), 7.31 (d, J = 8.4 Hz, 2H), 5.94 (t, J = 6.8 Hz, 1H), 3.28-3.17 (m, 1H), 2.90-2.75 (m, 1H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 151.1, 143.7, 136.0, 135.2, 133.8, 132.5, 129.5, 129.1, 128.8, 125.5, 124.9 (q, J_{CF} = 275.0 Hz), 121.9, 82.2 (q, J_{CF} = 3.0 Hz), 39.4 (q, J_{CF} = 29.0 Hz).
^{19}F NMR (376 MHz, $CDCl_3$) δ -63.1 (s, 3F).
HRMS (ESI) calcd. for $C_{16}H_{11}ClF_3N_3O_2Na$ [M+Na] 392.0384, found 392.0385.



4ua

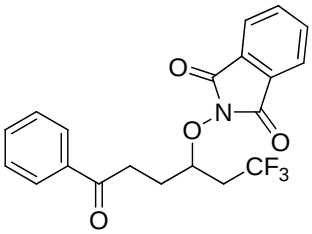
2-(3,3,3-Trifluoro-1-(4-methoxyphenyl)propoxy) isoindoline-1,3-dione (4ua)

White solid (73% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74-7.67 (m, 4H), 7.39 (d, *J* = 8.8 Hz, 2H), 6.85 (d, *J* = 8.8 Hz, 2H), 5.63 (t, *J* = 6.4 Hz, 1H), 3.77 (s, 3H), 3.12-3.04 (m, 1H), 2.80-2.72 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.3, 160.6, 134.4, 129.5, 128.5, 127.6, 125.0 (q, J_{CF} = 275.0 Hz), 123.4, 113.9, 82.0 (q, J_{CF} = 3.0 Hz), 55.1, 39.2 (q, J_{CF} = 29.0 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -63.3 (s, 3F).

HRMS (ESI) calcd. for $C_{18}H_{14}F_3NO_4Na$ [M+Na] 388.0767, found 388.0769.



4va

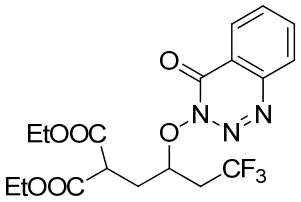
2-((1,1,1-Trifluoro-6-oxo-6-phenylhexan-3-yl)oxy) isoindoline-1,3-dione (4va)

White solid (78% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 7.2 Hz, 2H), 7.84-7.81 (m, 2H), 7.78-7.75 (m, 2H), 7.58 (d, *J* = 7.6 Hz, 1H), 7.49 (d, *J* = 7.6 Hz, 2H), 4.60-4.54 (m, 1H), 3.61-3.53 (m, 1H), 3.49-3.41 (m, 1H), 2.95-2.86 (m, 1H), 2.63-2.53 (m, 1H), 2.42-2.34 (m, 1H), 2.21-2.12 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 198.9, 164.0, 136.8, 134.8, 133.1, 128.7, 128.6, 128.1, 125.4 (q, J_{CF} = 275.0 Hz), 123.7, 82.1 (q, J_{CF} = 3.0 Hz), 38.5 (q, J_{CF} = 29.0 Hz), 33.7, 27.6.

^{19}F NMR (376 MHz, $CDCl_3$) δ -63.3 (s, 3F).

HRMS (ESI) calcd. for $C_{20}H_{17}F_3NO_4$ [M+H] 392.1104, found 392.1102.

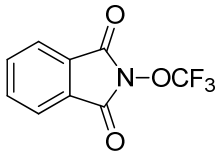


4wc

Diethyl 2-(4,4,4-trifluoro-2-((4-oxobenzo[d][1,2,3]triazin-3(4H)-yl)oxy)butyl) mal onate (4wc)

Yellow oil (71% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 8.0, 1H), 8.21 (d, *J* = 8.0 Hz, 1H), 8.03-7.98 (m, 1H), 7.86-7.82 (m, 1H), 4.88-4.82 (m, 1H), 4.31-4.21 (m, 5H), 3.08-3.00 (m, 1H), 2.71-2.56 (m, 2H), 2.46-2.39 (m, 1H), 1.32-1.27 (m, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 169.1, 168.7, 151.39, 143.9, 135.3, 132.7, 128.9, 125.6, 125.1 (q, J_{CF} = 275.0 Hz), 122.1, 80.9 (q, J_{CF} = 3.0 Hz), 61.8, 47.8, 33.1 (q, J_{CF} = 29.0 Hz), 32.8, 14.0.
^{19}F NMR (376 MHz, $CDCl_3$) δ -63.1 (s, 3F).
HRMS (ESI) calcd. for $C_{18}H_{20}F_3N_3O_6Na$ [M+Na] 454.1196, found 454.1197.

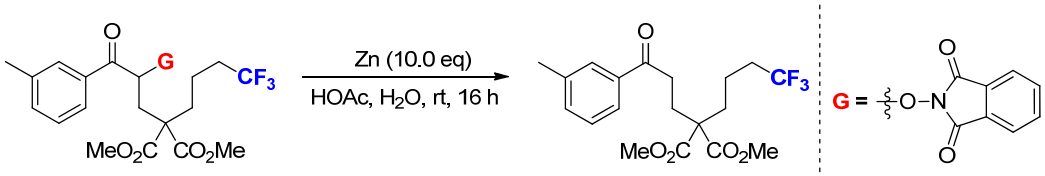


5

2-(Trifluoromethoxy)isoindoline-1,3-dione (5)
White solid (45% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (dd, J = 5.6, 3.2 Hz, 2H), 7.87 (dd, J = 5.2, 3.2 Hz, 2H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 161.5, 135.5, 128.6, 124.5. 122.1 (q, J_{CF} = 267.0 Hz);
^{19}F NMR (376 MHz, $CDCl_3$) δ -65.2 (s, 3F).
HRMS (ESI) calcd. for $C_{10}H_8F_3NO_4Na$ [M+MeOH+Na] 286.0298, found 286.0297.

Experiments for transformations of compounds 4ga and 4aa

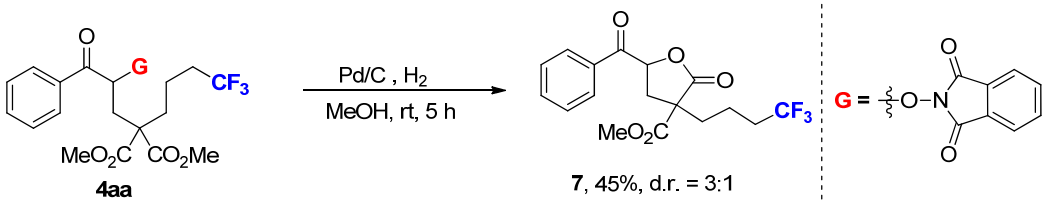
1)



4ga **6**,~100% yield

Procedure[6]: To a flame-dried flask equipped with a magnetic stir bar were added **4ga** (57.2 mg, 0.1 mmol), activated Zinc powder (66.0 mg, 1.0 mmol) in a mixture of AcOH/H_2O (2.0 ml/0.2 ml) and then allowed to stir at rt under air for 16 h. The crude reaction mixture was diluted with H_2O (20 mL), extracted with CH_2Cl_2 (3 x 20 mL), washed with brine, dried ($MgSO_4$), and concentrated. The resultant residue was purified by flash chromatography (ethyl acetate/petroleum ether = 1/10-1/6) to afford dimethyl 2-(3-oxo-3-(m-tolyl) propyl)-2-(4,4,4-trifluorobutyl) malonate (**6**) (41.1 mg, ~100% yield) as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74-7.72 (m, 2H), 7.38-7.32 (m, 2H), 3.73 (s, 6H), 2.96 (d, J = 8.0 Hz, 2H), 2.40 (s, 3H), 2.33 (d, J = 8.0 Hz, 2H), 2.15-1.97 (m, 4H), 1.56-1.48 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.8, 171.5, 138.5, 136.6, 134.0, 128.5, 128.5, 126.8 (q, J_{CF} = 275.0 Hz), 125.2, 56.9, 52.6, 33.8 (q, J_{CF} = 29.0 Hz), 33.8, 33.1, 27.5, 21.3, 17.2 (q, J_{CF} = 3.0 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.2 (s, 3F). HRMS (ESI) calcd. for $C_{19}H_{23}O_5F_3Na$ [M+Na] 411.1390, found 411.1389.

2)

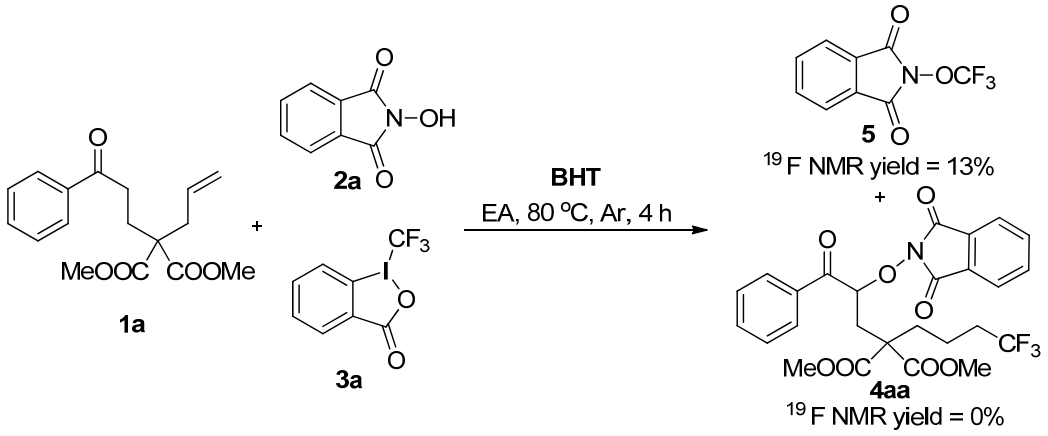


Procedure[7]: To a flame-dried flask equipped with a magnetic stir bar were added **4aa** (55.8 mg, 0.1 mmol), 10 % Pd on carbon (25.0 mg) in MeOH (15 mL). The flask was evacuated and refilled with H_2 four times, and then allowed to stir at rt under 1 atm H_2 for 5 h. The reaction mixture was then filtered through Celite and concentrated. The resultant residue was purified by flash chromatography (ethyl acetate/petroleum ether = 1/12-1/8) to afford methyl 5-benzoyl-2-oxo-3-(4,4,4-trifluorobutyl) tetrahydrofuran-3-carboxylate (**7**) (16.1 mg, d.r. = 3:1; 45% yield) as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, J = 7.6 Hz, 2H), 7.65 (t, J = 7.6 Hz, 1H), 7.53 (t, J = 7.6 Hz, 2H), 5.76 (dd, J = 9.2, 7.2 Hz, 1H), 3.86 (s, 3H), 3.03 (dd, J = 13.6, 7.2 Hz, 1H), 2.46 (dd, J = 13.6, 9.2 Hz, 1H), 2.15-2.07 (m, 2H), 1.71-1.49 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.2, 172.5, 169.3, 134.5, 133.9, 129.1, 129.0, 126.6 (q, J_{CF} = 275.0 Hz), 76.9, 54.9, 53.7, 34.0, 33.6 (q, J_{CF} = 29.0 Hz), 33.3, 17.7 (q, J_{CF} = 3.0 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.3(s, 3F). HRMS (ESI) calcd. for $C_{17}H_{18}O_5F_3$ [M+H] 359.1101, found 359.1102.

Experiments for mechanistic studies

1) Control experiments

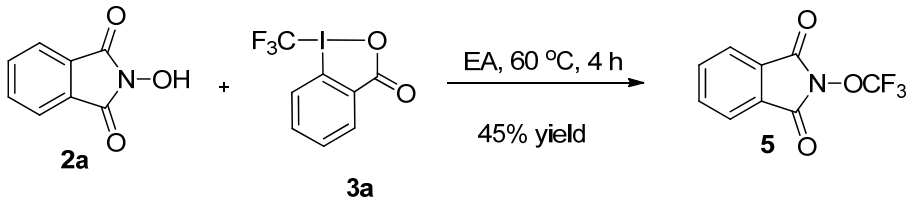
Reaction of BHT, NHPI (2a) and Togni's reagent 3a with 1a[8]



Procedure: To a flame-dried Schlenk tube equipped with a magnetic stir bar were added **1a** (25.2 mg, 0.1 mmol), **2a** (32.6 mg, 0.2 mmol), **3a** (63.2 mg, 0.2 mmol) and BHT (41.3 mg, 0.20 mmol). The tube was evacuated and backfilled with argon for three times, and ethyl acetate (1.0 mL) was added *via* syringe. The sealed tube was stirred at 80 °C for 4 h. Solvent was removed under reduced pressure, and the residue

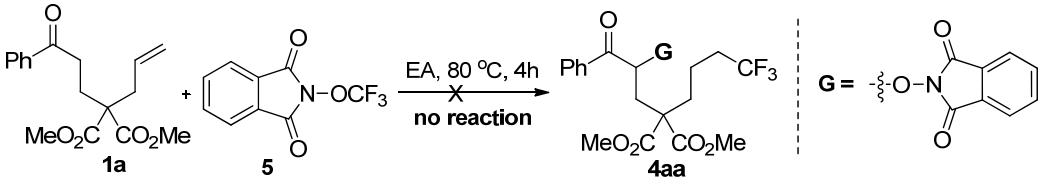
was dissolved in $CDCl_3$, then α,α,α-trifluorotoluene (29.2 mg, 0.2 mmol) was added as internal standard. ^{19}F NMR analysis of the mixture showed that **5** was formed in 13% yield and **4aa** was formed in 0% yield.

Reaction of NHPI (2a) with Togni's reagent 3a[4]



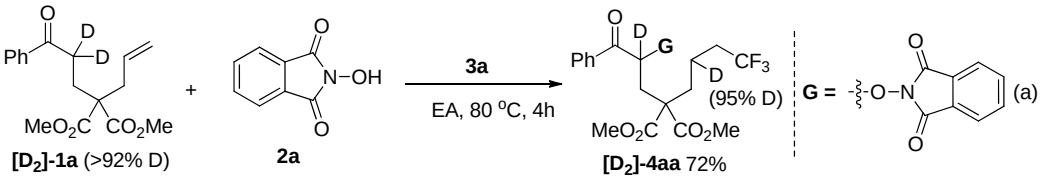
Procedure: To a flame-dried Schlenk tube equipped with a magnetic stir bar were added **2a** (16.3 mg, 0.1 mmol), and Togni's reagent **3a** (316.2 mg, 0.1 mmol). The tube was evacuated and backfilled with argon for three times, and then ethyl acetate (1.0 mL) was added *via* syringe. The sealed tube was stirred at 80 °C for 4 h. Solvent was removed under reduced pressure, and the residue was purified by flash chromatography on silica gel (ethyl acetate/petroleum ether = 1/16-1/10) to give the PINO-CF_3 **5** in 45% yield (white solid).

Reaction of 5 with Togni's reagent 1a



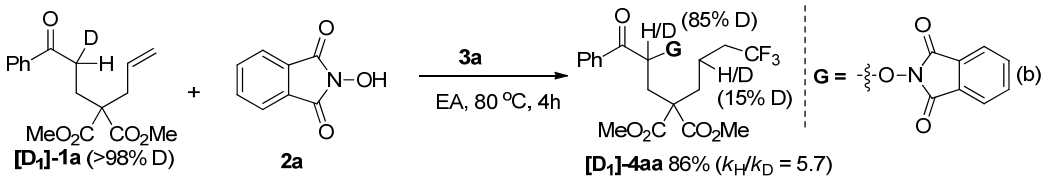
Procedure: To a flame-dried Schlenk tube equipped with a magnetic stir bar were added **1a** (25.2 mg, 0.1 mmol) and **5** (23.1 mg, 0.1 mmol). The tube was evacuated and backfilled with argon for three times, and then ethyl acetate (1.0 mL) was added *via* syringe. The sealed tube was stirred at 80 °C for 4 h and cooled to room temperature. However, TLC shows that no reaction occurred.

2) D-labeling experiments



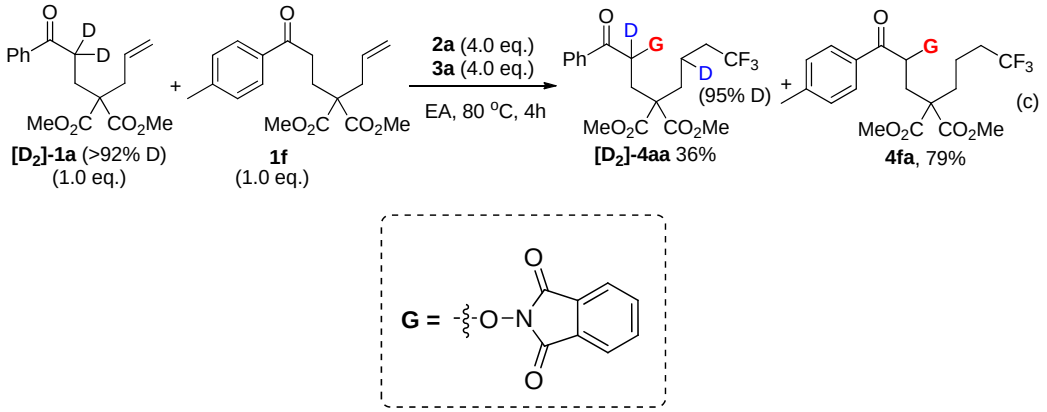
Procedure: To a flame-dried Schlenk tube equipped with a magnetic stir bar were added [**D_2**]**-1a** (153.0 mg, 0.5 mmol), Togni's reagent **3a** (316.0 mg, 1.0 mmol) and **2a (NHPI)** (163.0 mg, 1.0 mmol). The tube was evacuated and backfilled with argon for three times, and ethyl acetate (5.0 mL) was added *via* syringe. The tube was stirred at 80 °C for 4 h. Solvent was removed under reduced pressure, and the crude residue was purified by silica gel column chromatography (ethyl acetate/petroleum ether =

1/8-1/2) to give [**D$_2$**]-**4aa** in 72% yield (white solid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, J = 7.2, 2H), 7.82-7.79 (m, 2H), 7.76-7.73 (m, 2H), 7.63-7.59 (m, 1H), 7.50 (d, J = 7.6, 2H), 5.89 (t, J = 5.6 Hz, 0.05H), 3.70 (s, 3H), 3.57 (s, 3H), 2.79 (d, J = 15.6 Hz, 1H), 2.63 (d, J = 15.6 Hz, 1H), 2.28-2.09 (m, 4H), 1.58-1.47 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.8, 171.0, 170.6, 163.4, 134.7, 134.6, 134.0, 129.3, 128.8, 128.7, 126.8 (q, J_{CF} = 275.0 Hz), 123.7, 82.7, 55.9, 52.9, 52.7, 31.7 (q, J_{CF} = 29.0 Hz), 33.0, 32.8, 17.25(m). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.3 (s, 3F). HRMS (ESI) m/z calcd. for $C_{26}H_{22}D_2F_3NO_8Na$ [M+Na] 560.1472, found 560.1471.



Procedure: To a flame-dried Schlenk tube equipped with a magnetic stir bar were added [**D$_1$**]-**1a** (152.5 mg, 0.5 mmol), Togni's reagent **3a** (316.0 mg, 1.0 mmol) and **2a (NHPI)** (163.0 mg, 1.0 mmol). The tube was evacuated and backfilled with argon for three times, and ethyl acetate (5.0 mL) was added *via* syringe. The tube was stirred at 80 °C for 4 h. Solvent was removed under reduced pressure, and the crude residue was purified by silica gel column chromatography (ethyl acetate/petroleum ether = 1/8-1/2) to give [**D$_1$**]-**4aa** in 86% yield (white solid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, J = 7.2, 2H), 7.82-7.79 (m, 2H), 7.76-7.73 (m, 2H), 7.63-7.58 (m, 1H), 7.50 (t, J = 8.0, 2H), 5.90 (t, J = 5.6 Hz, 0.15H), 3.70 (s, 3H), 3.57 (s, 3H), 2.80 (d, J = 15.2 Hz, 1H), 2.64 (d, J = 15.2 Hz, 1H), 2.53-2.11 (m, 4H), 1.60-1.47 (m, 1.85H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.8, 170.9, 170.6, 163.4, 134.7, 134.6, 134.0, 129.3, 128.8, 128.6, 126.8 (q, J_{CF} = 275.0 Hz), 123.7, 83.0, 82.6, 55.8, 52.9, 52.7, 31.7 (q, J_{CF} = 29.0 Hz), 31.64 (q, J_{CF} = 29.0 Hz), 32.93, 32.86, 17.30 (q, J_{CF} = 3.0 Hz). HRMS (ESI) m/z calcd. for $C_{26}H_{23}DF_3NO_8Na$ [M+Na] 559.1409, found 559.1409.

3) Crossover experiment



Procedure: To a flame-dried Schlenk tube equipped with a magnetic stir bar were added [**D$_2$**]-**1a** (76.5 mg, 0.25 mmol), **1f** (82.0 mg, 0.25 mmol), Togni's reagent **3a**

(316.0 mg, 1.0 mmol) and **2a (NHPI)** (163.0 mg, 1.0 mmol). The tube was evacuated and backfilled with argon for three times, and ethyl acetate (5.0 mL) was added *via* syringe. The tube was stirred at 80 °C for 4 h. Solvent was removed under reduced pressure, and the crude residue was purified by silica gel column chromatography (ethyl acetate/petroleum ether = 1/8-1/2) to give [**D_2]-4aa** and **4fa** in 36% and 79% yield, respectively.

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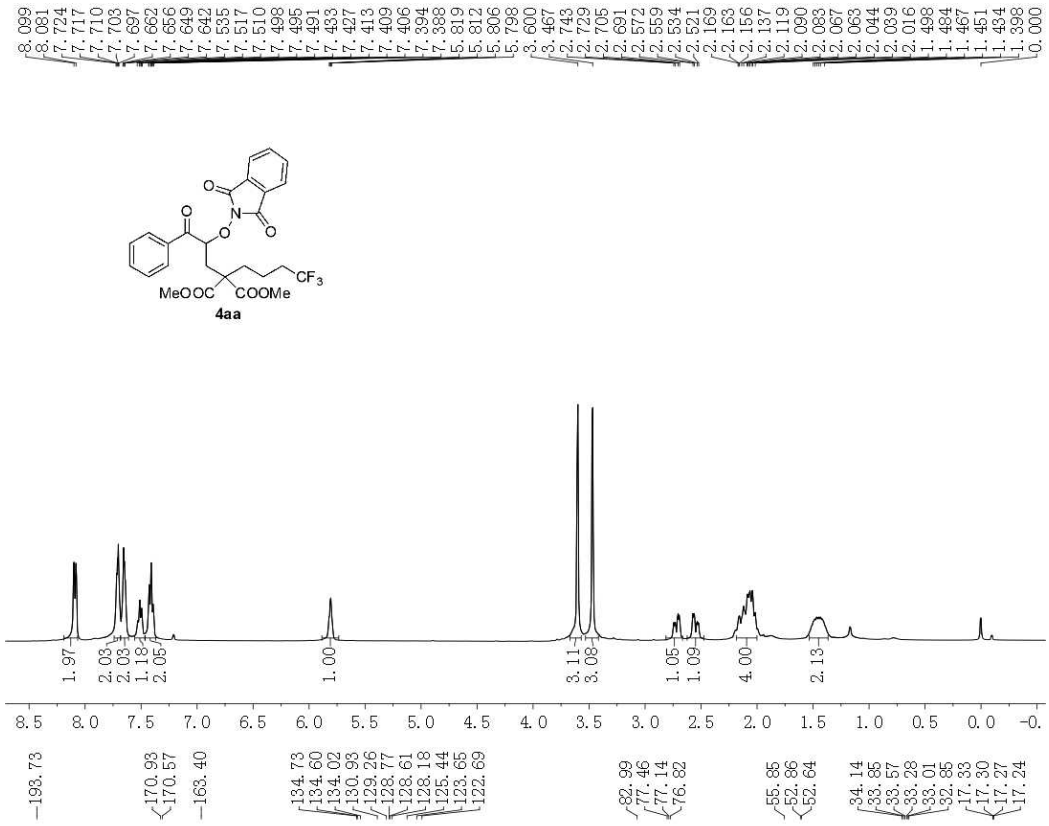
NMR spectra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MeOOC COOMe
CF3
4aa
1.97 2.03 2.03 1.18 2.05 1.00 3.11 3.08 1.05 1.09 4.00 2.13
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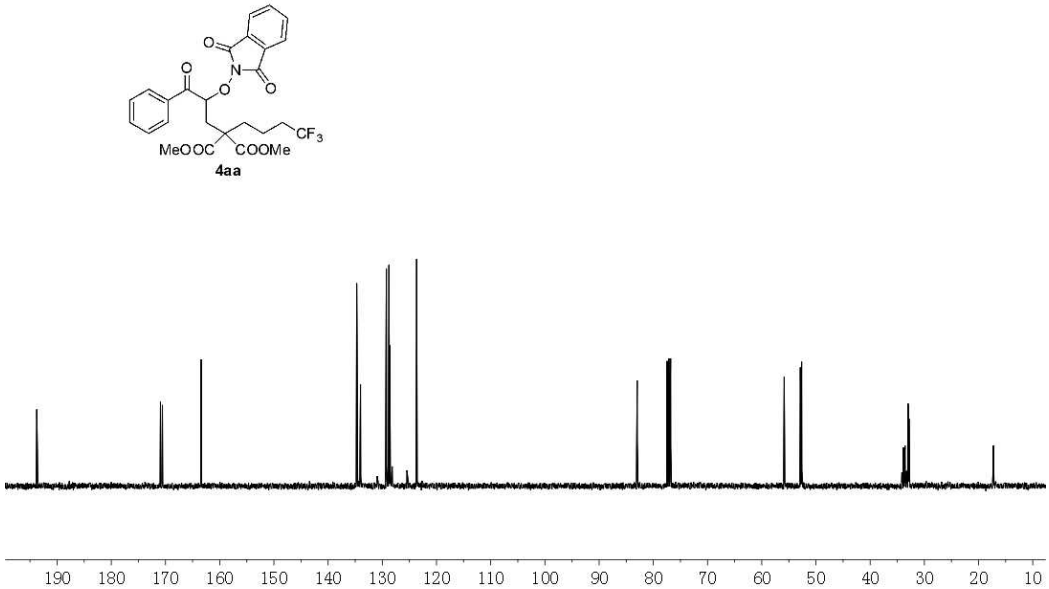
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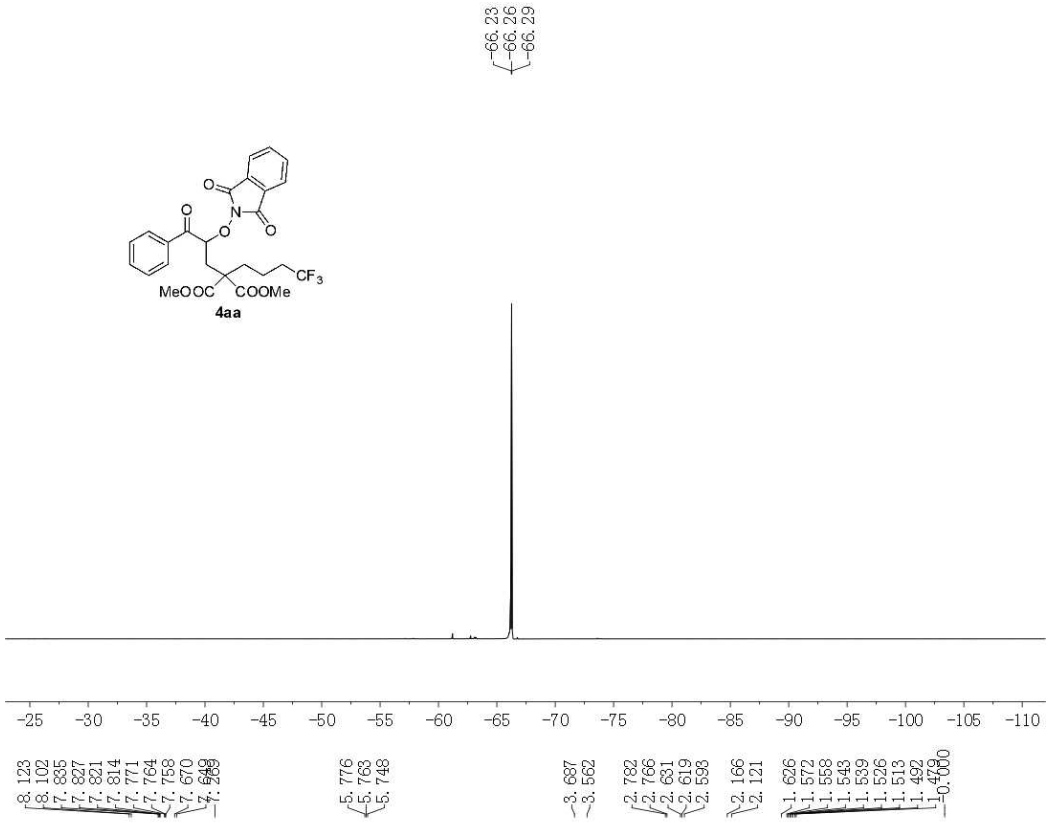
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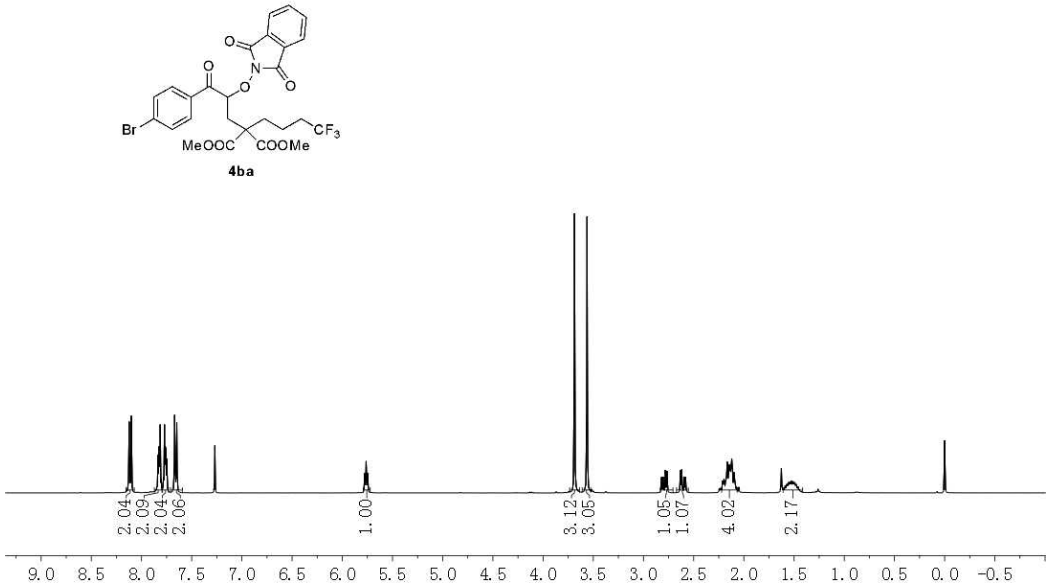
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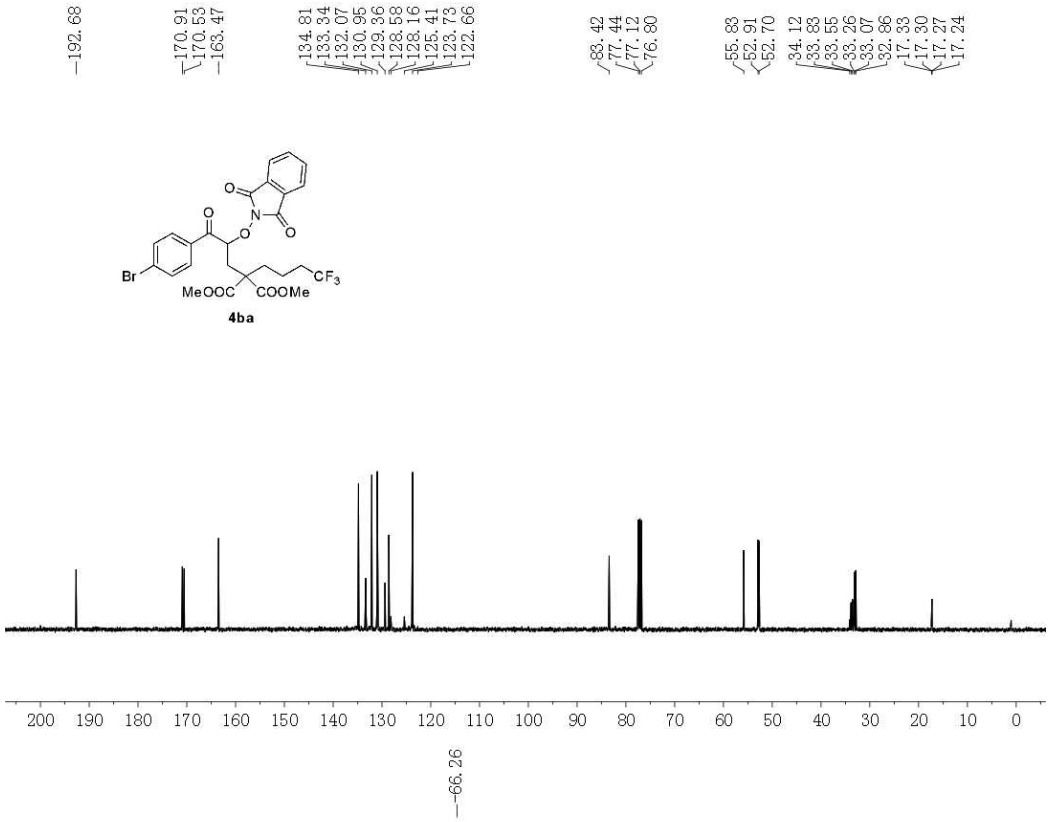
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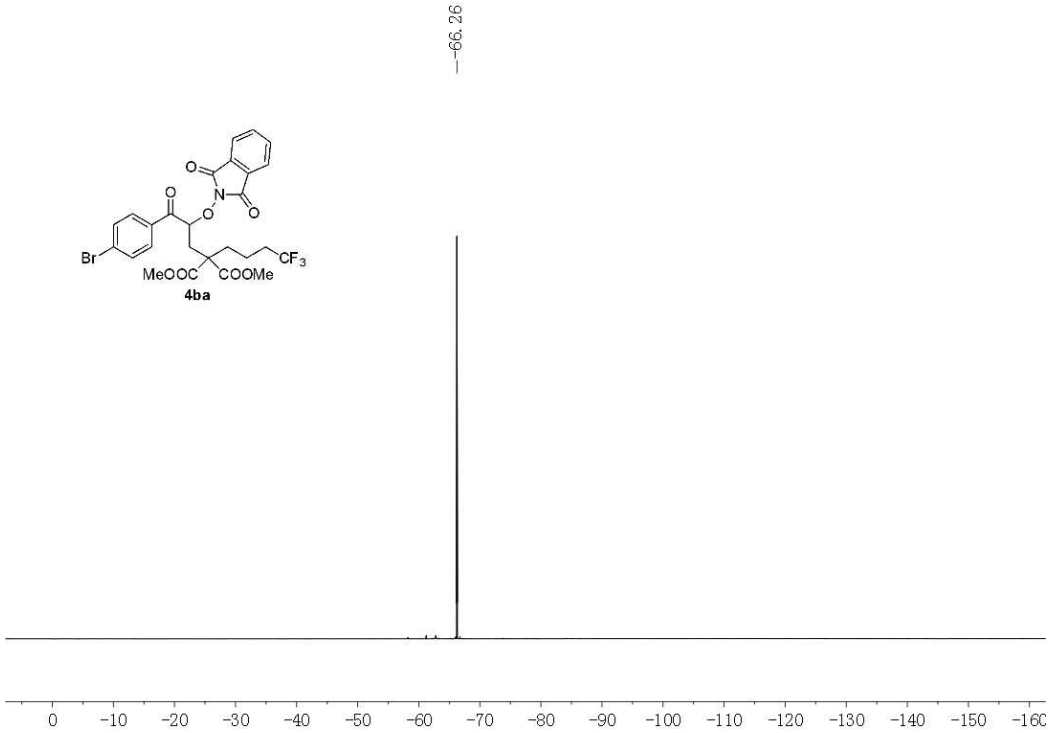
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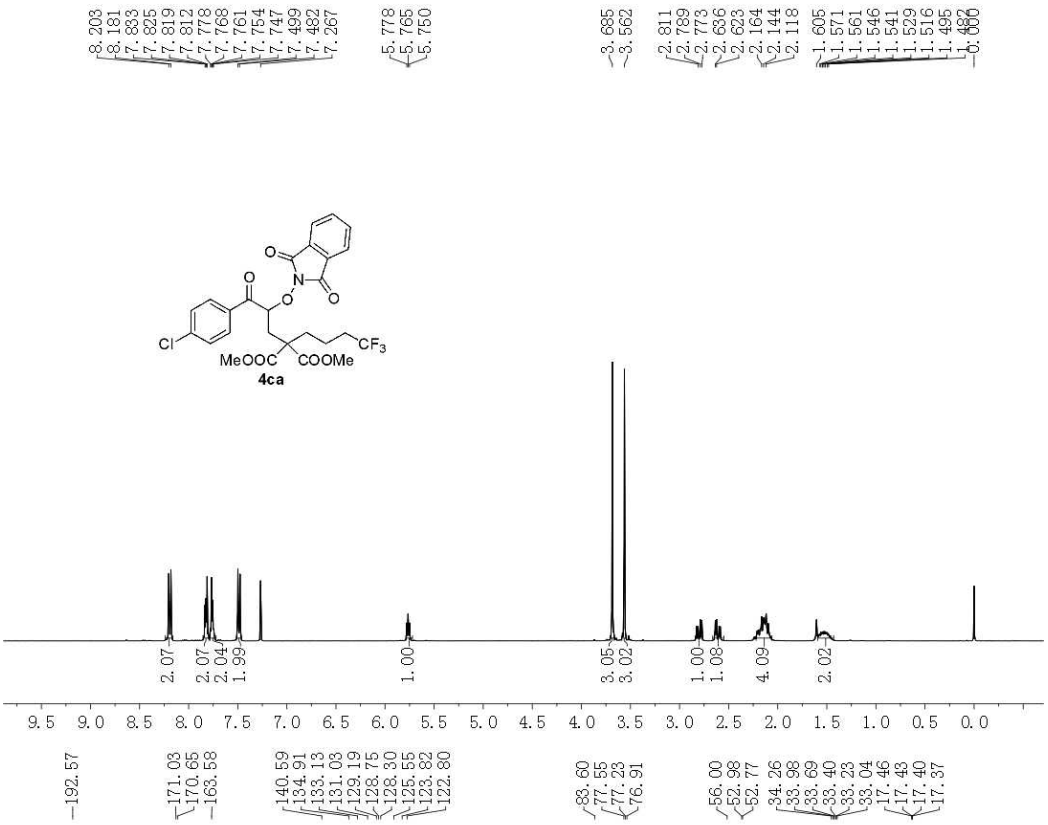
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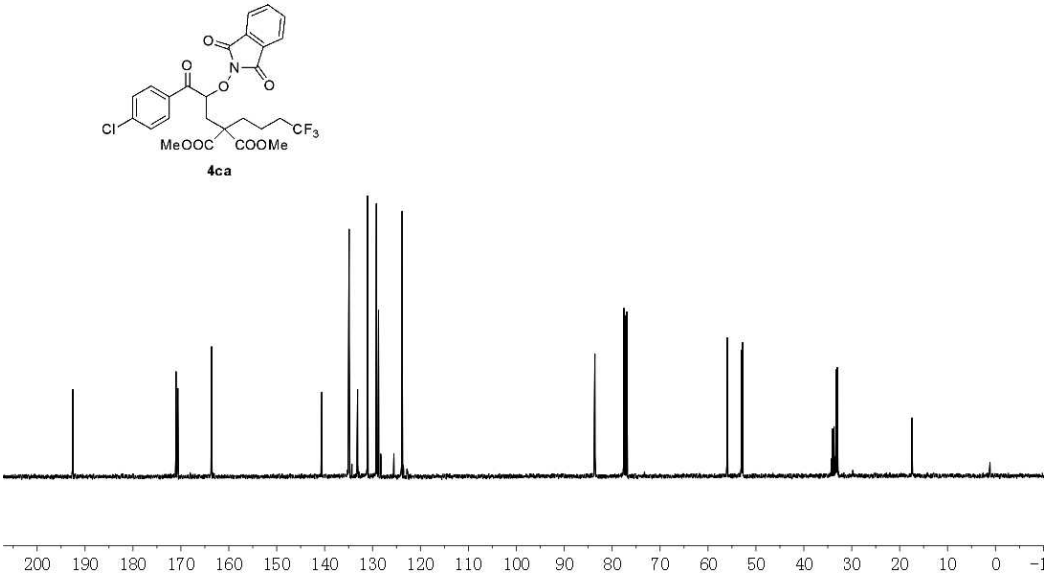
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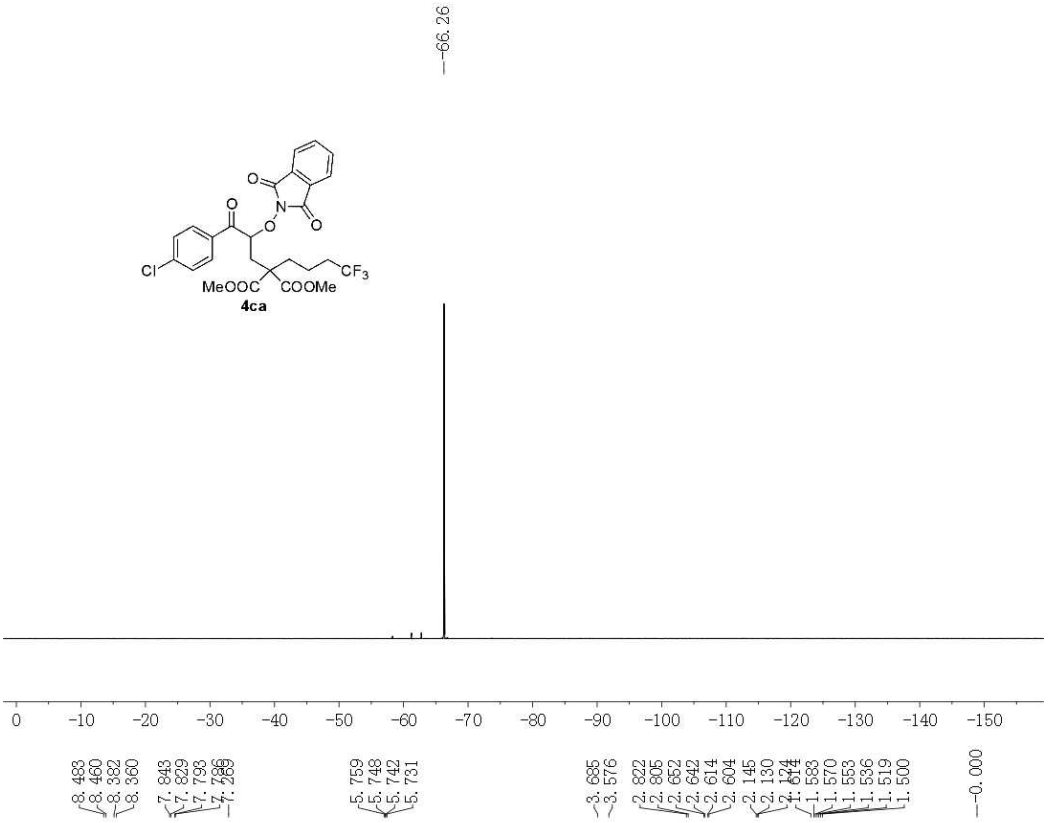
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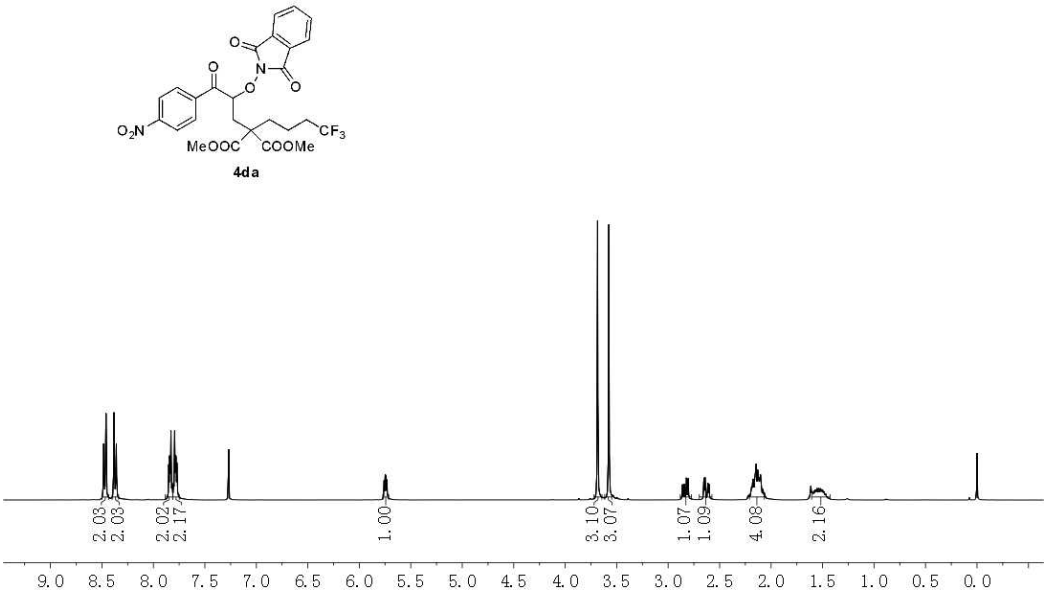
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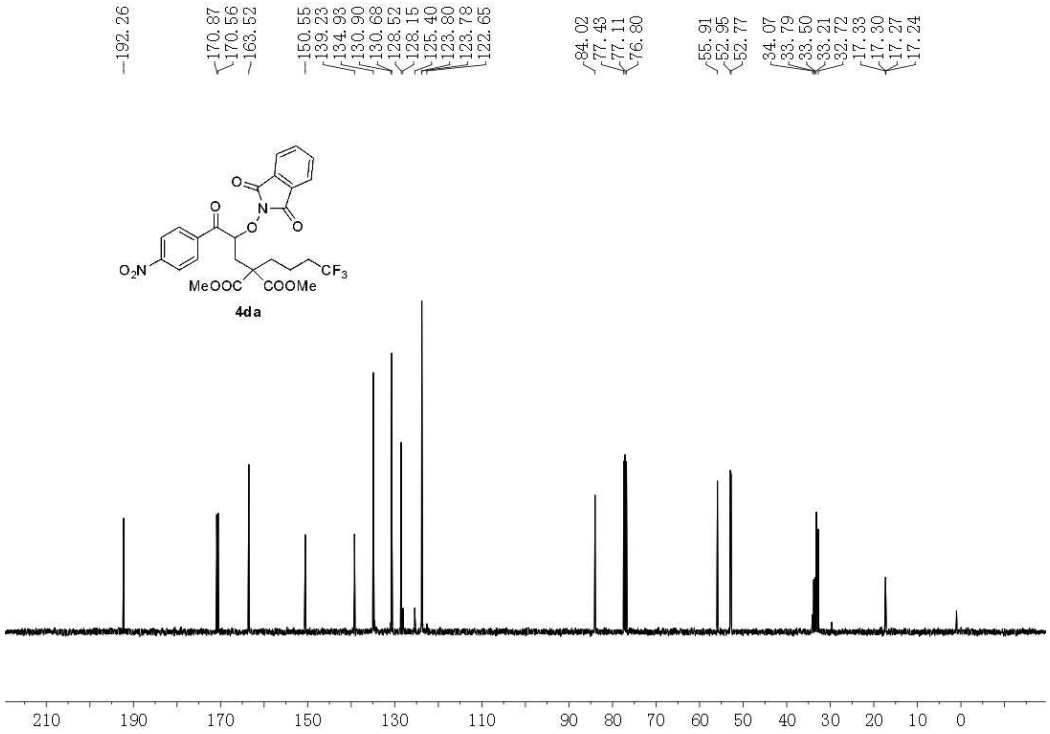
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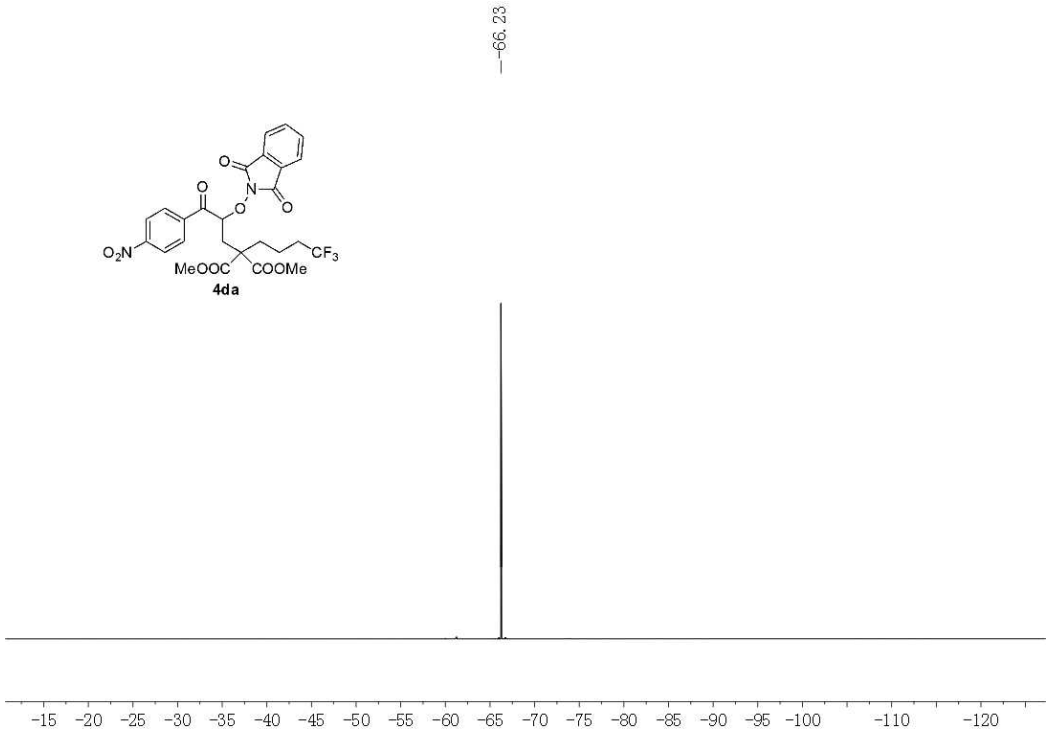
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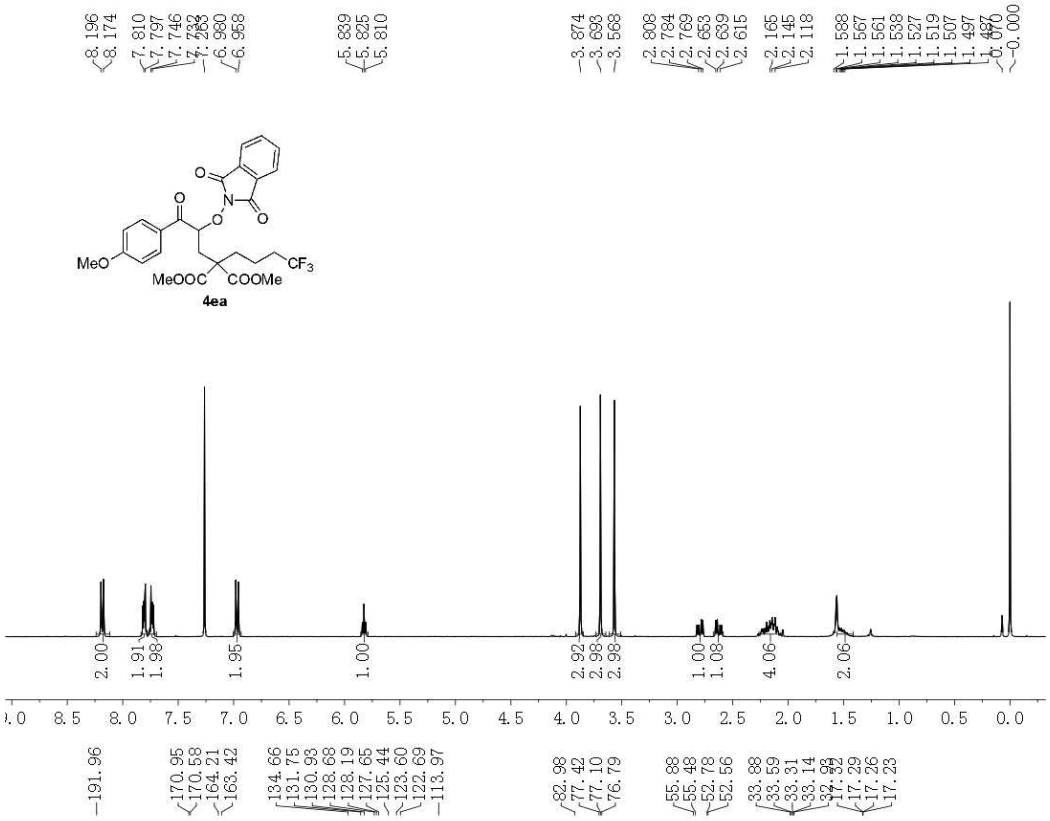
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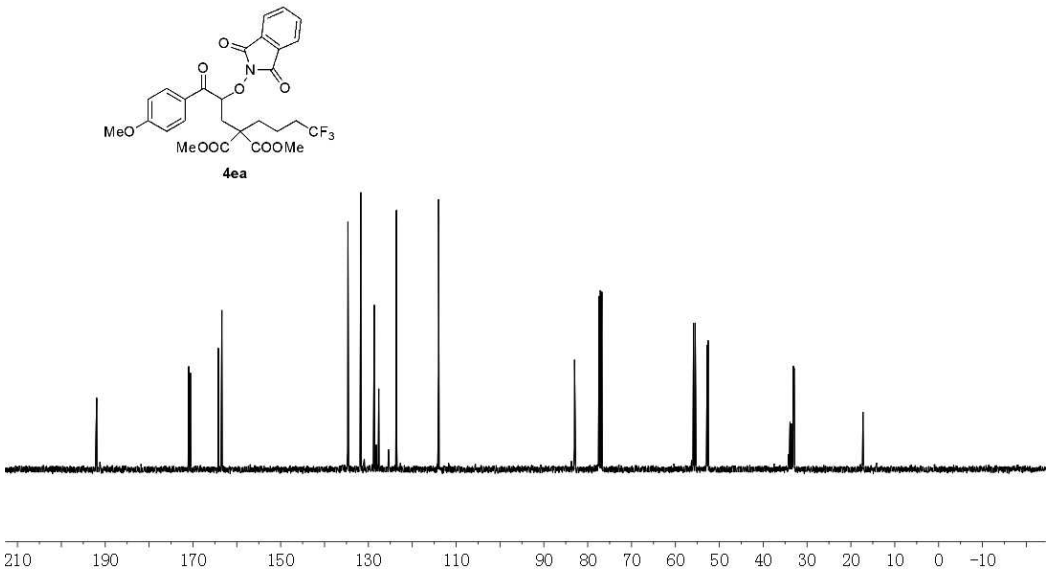
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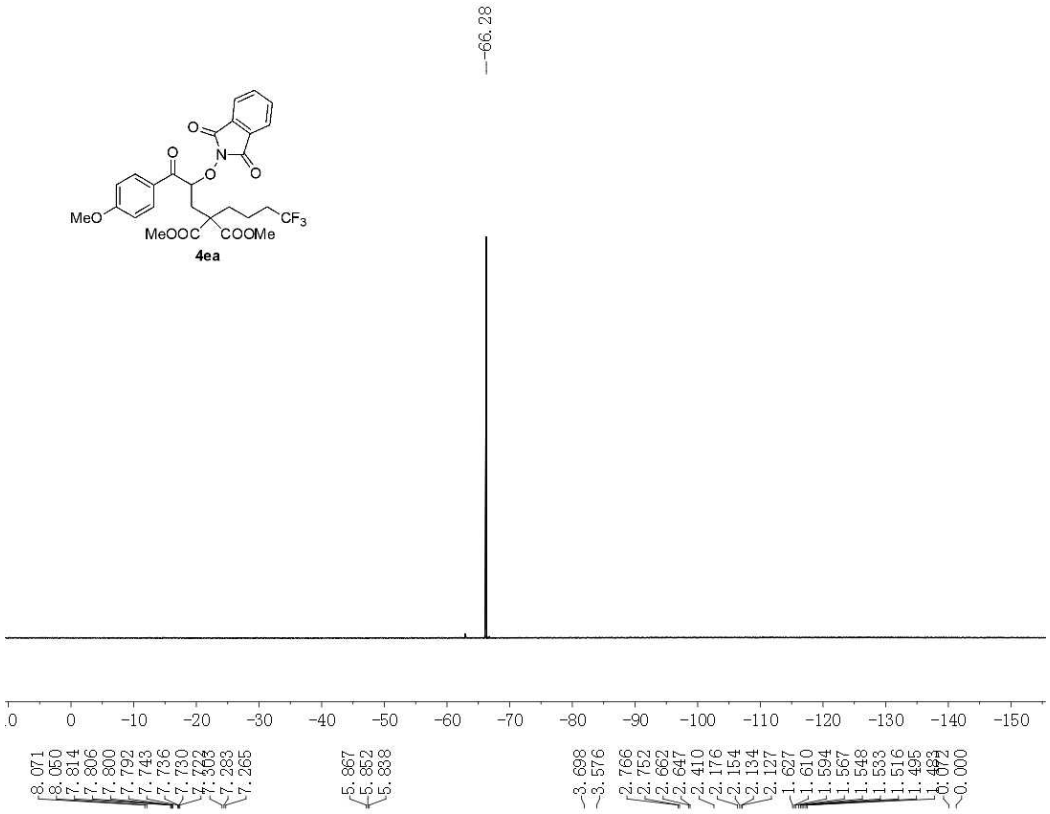
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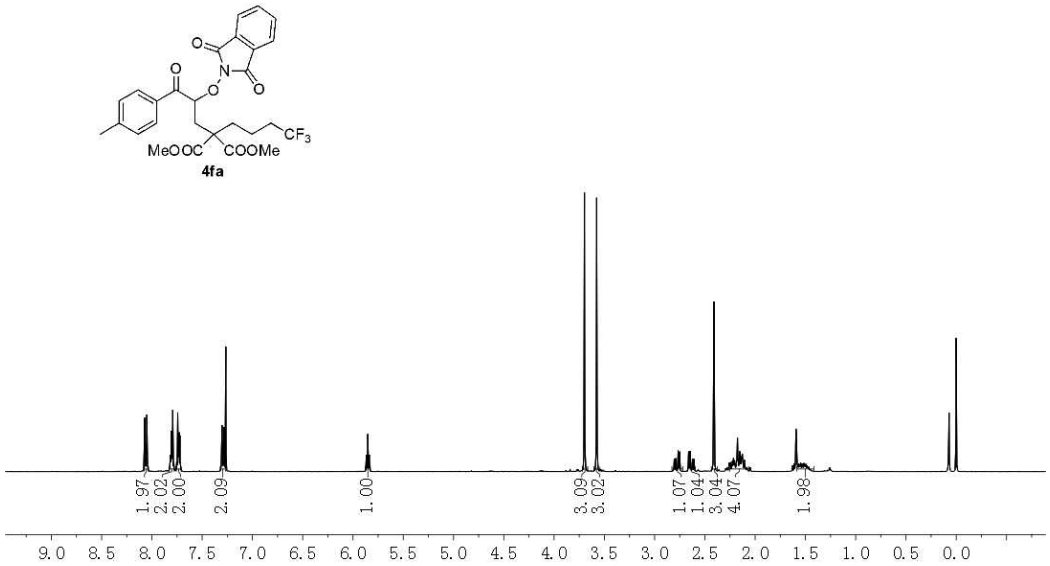
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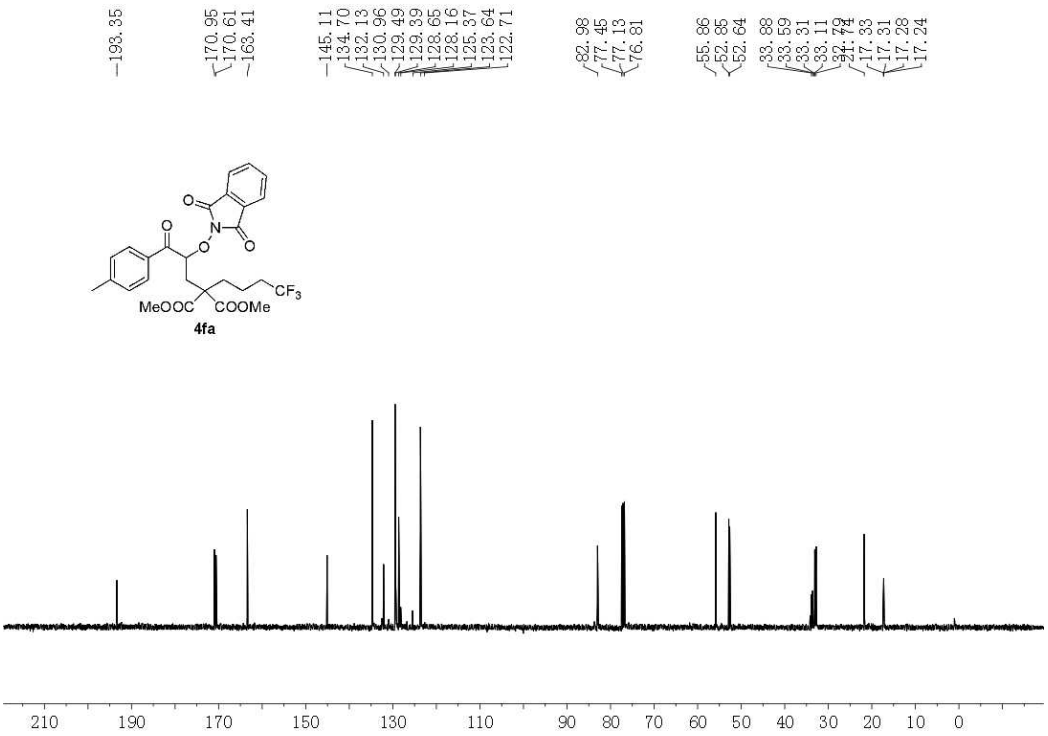
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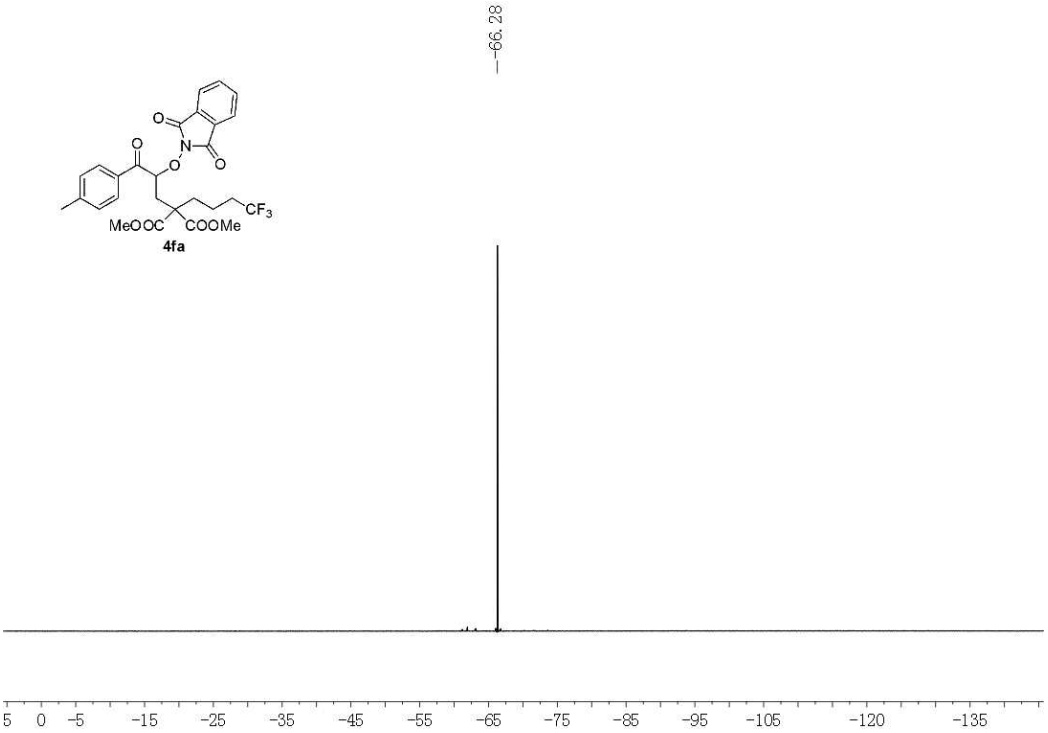
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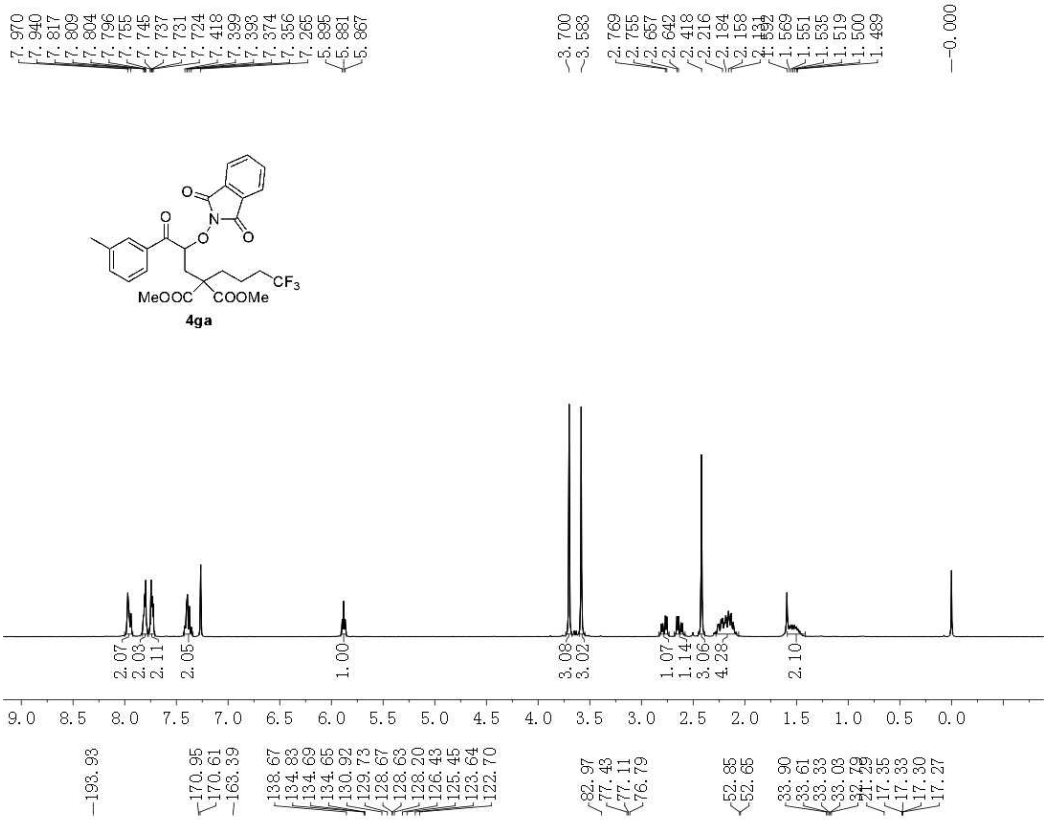
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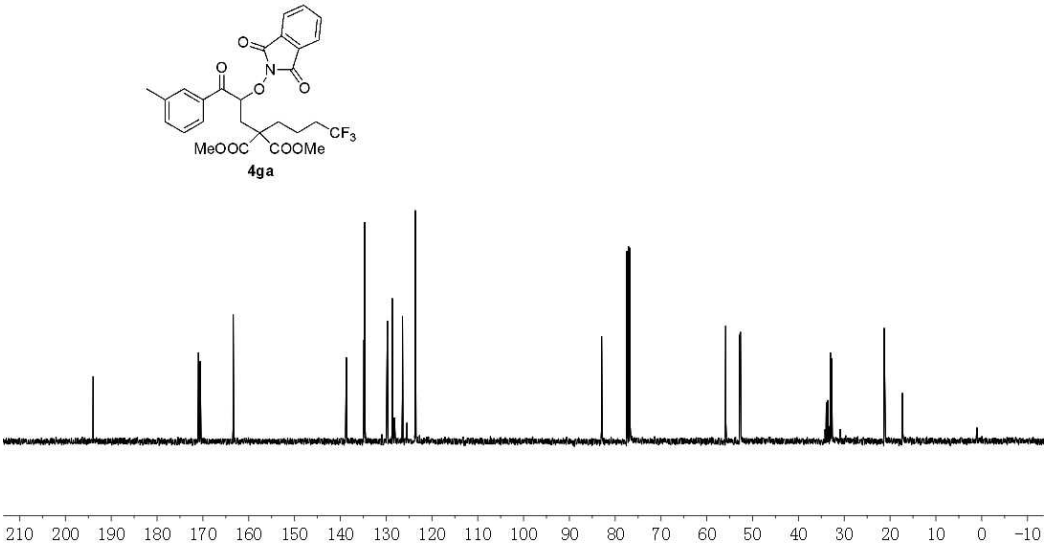
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MeOOC
COOMe
CF3

4ga

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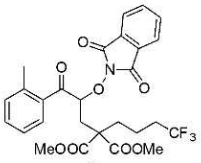
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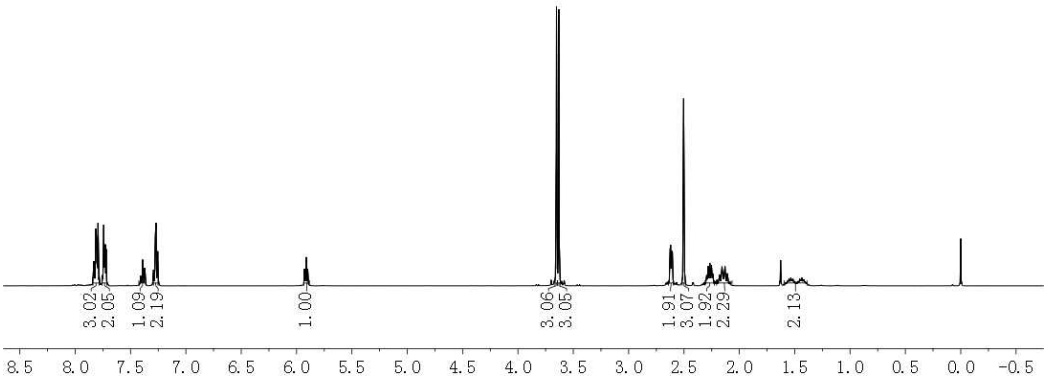
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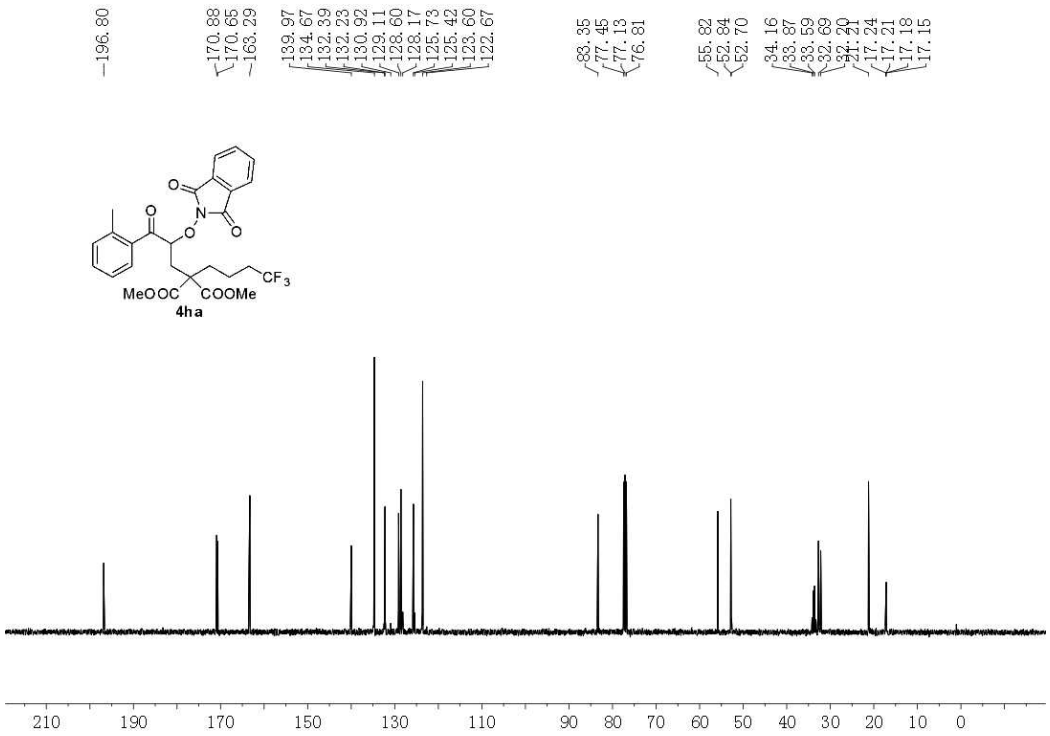
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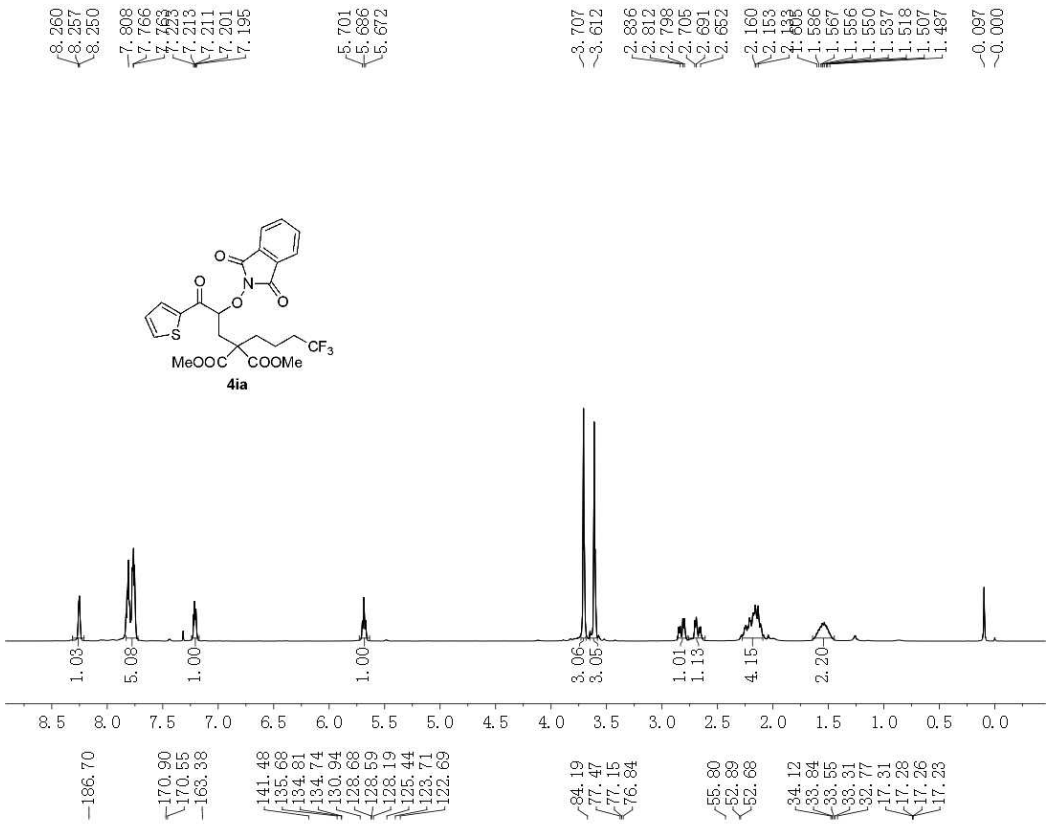
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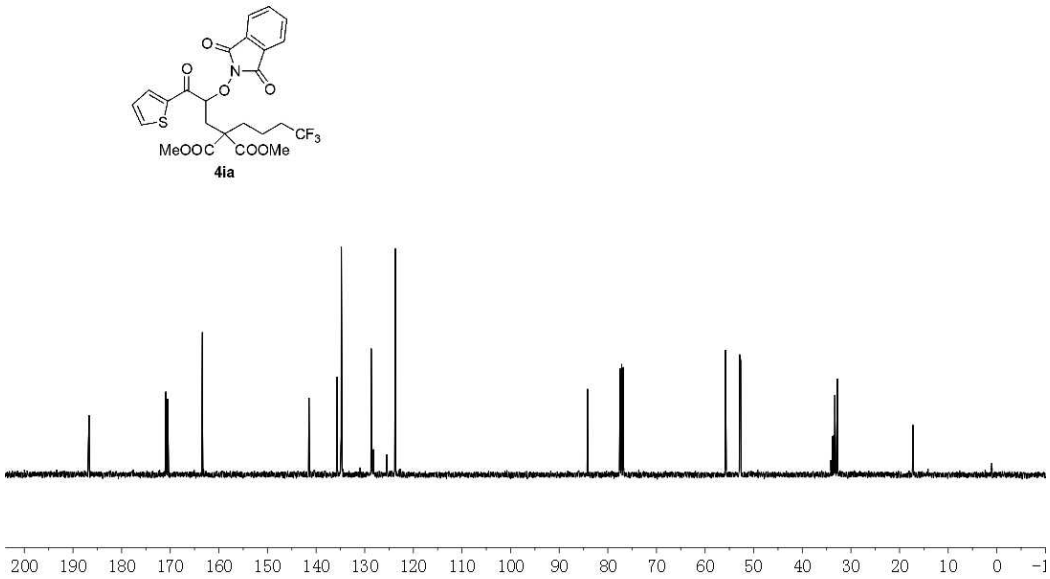
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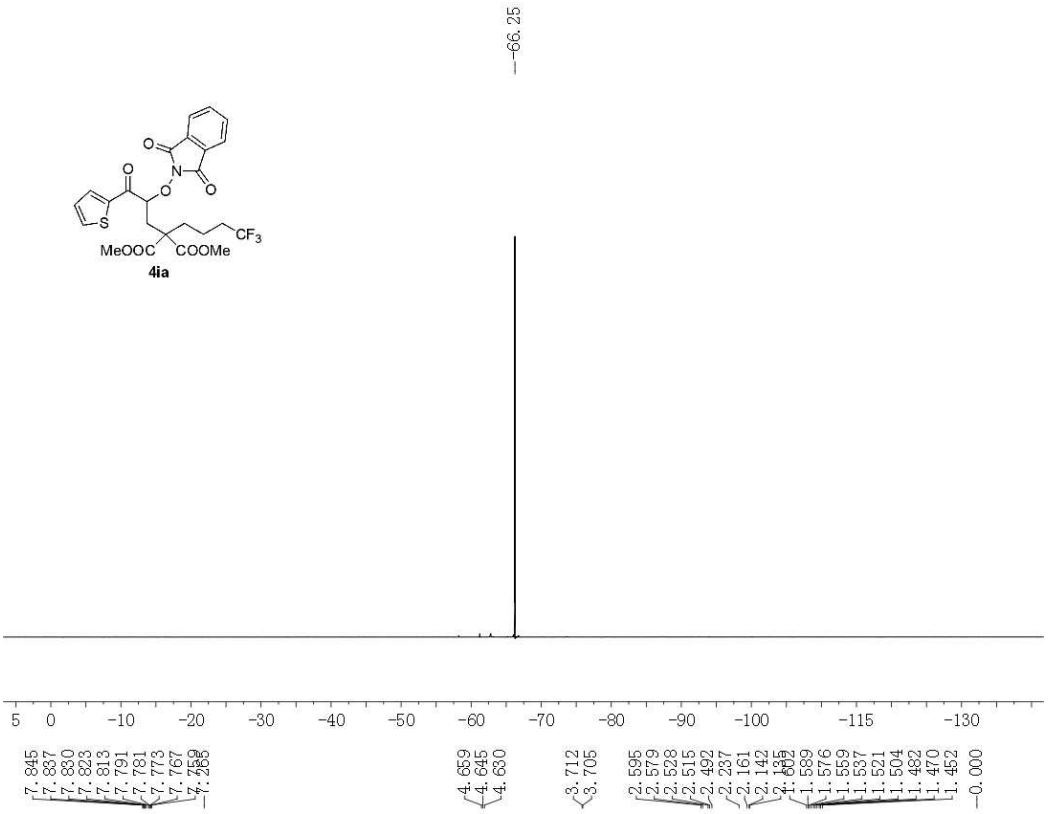
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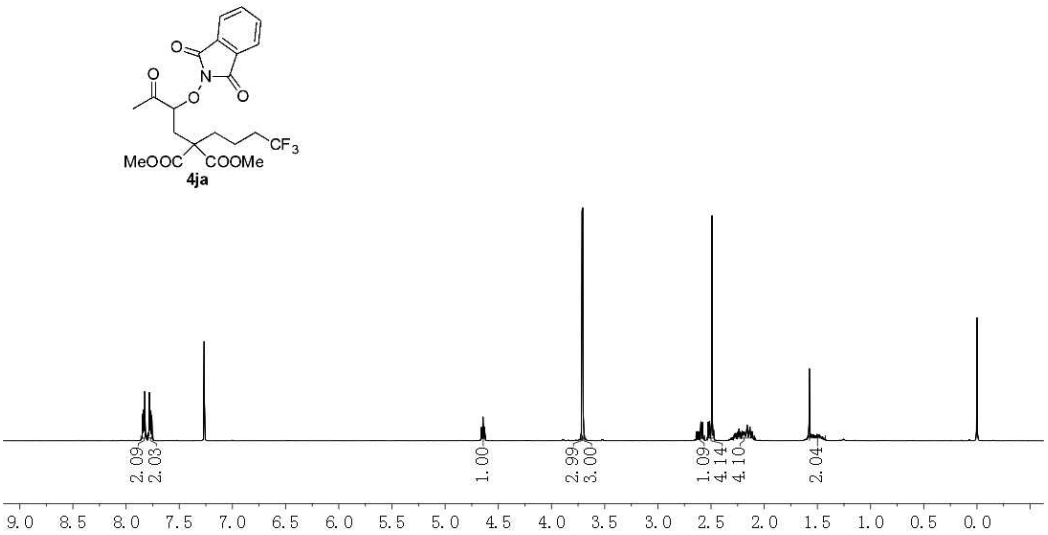
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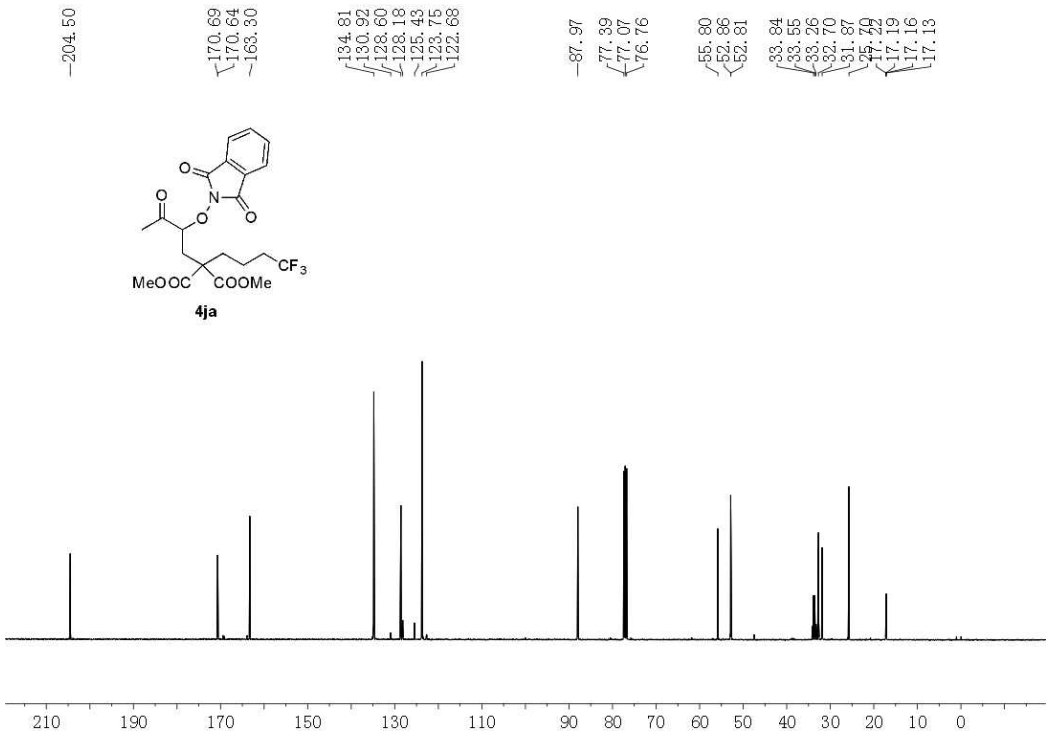
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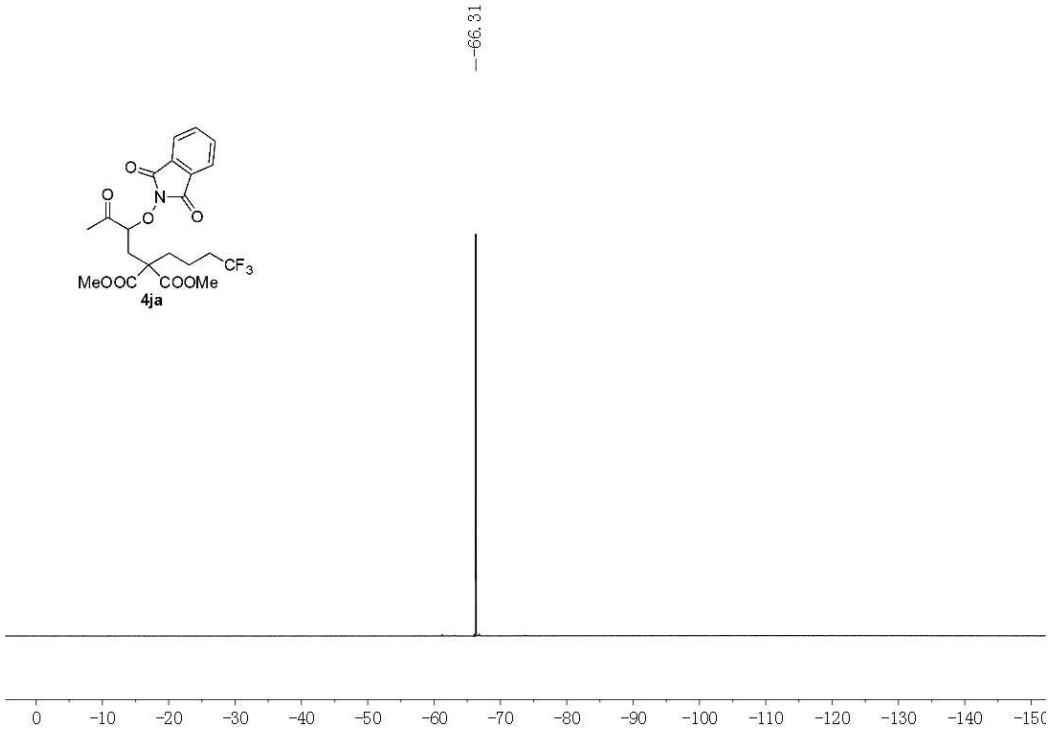
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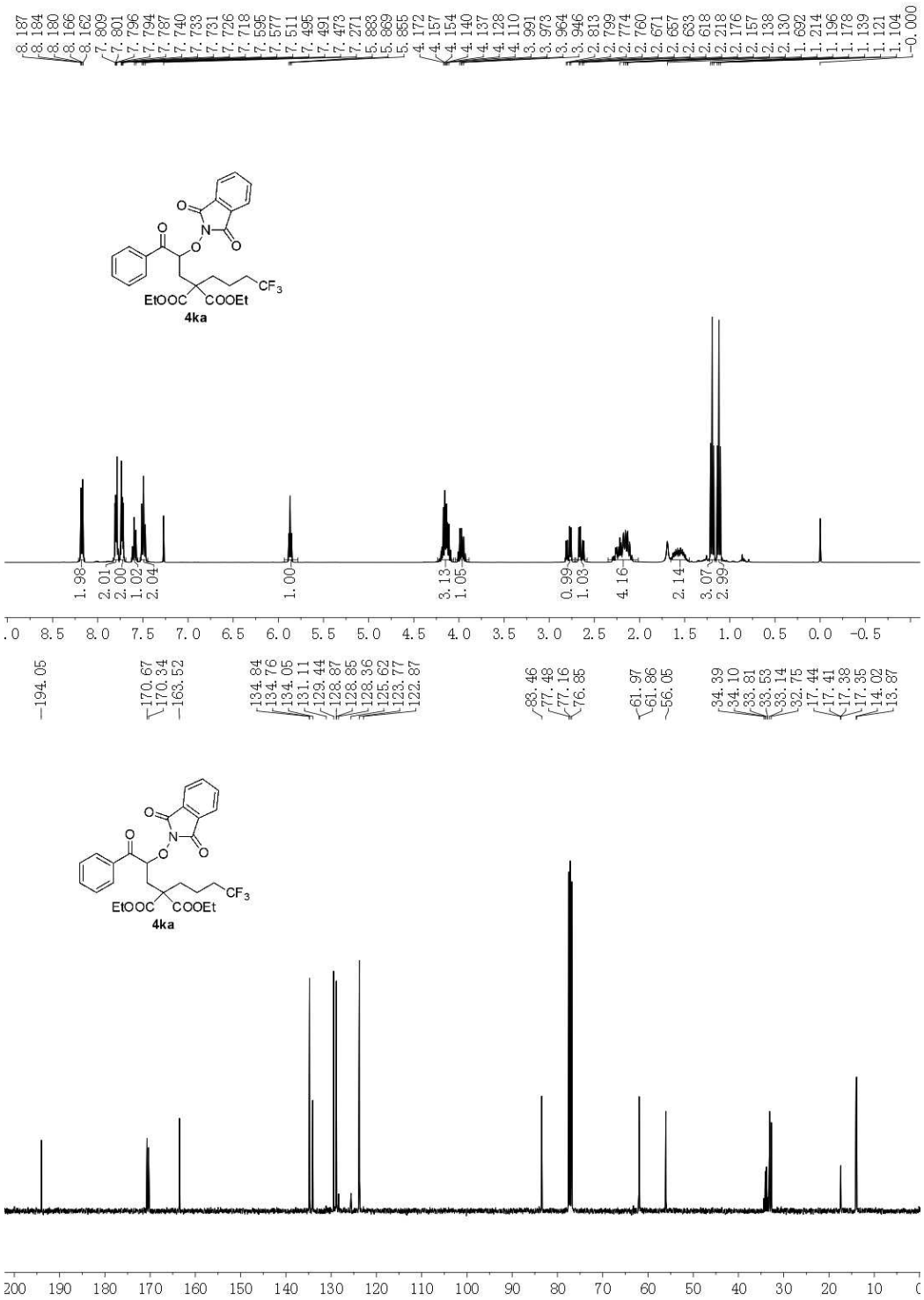
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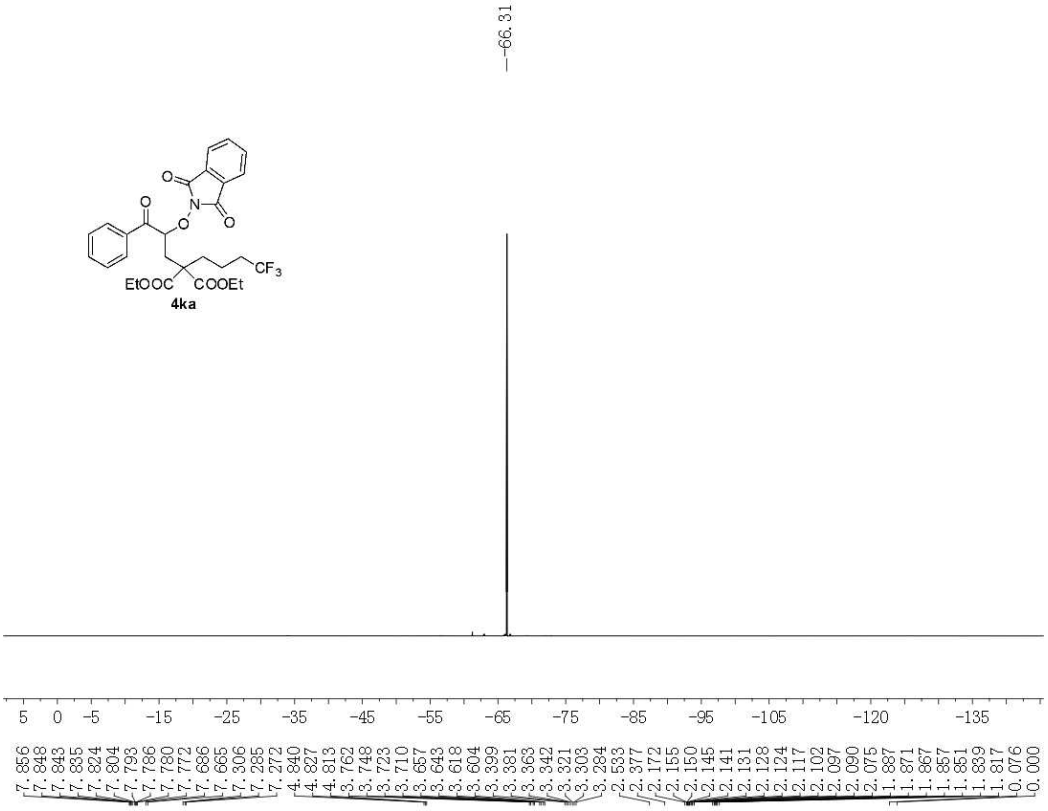
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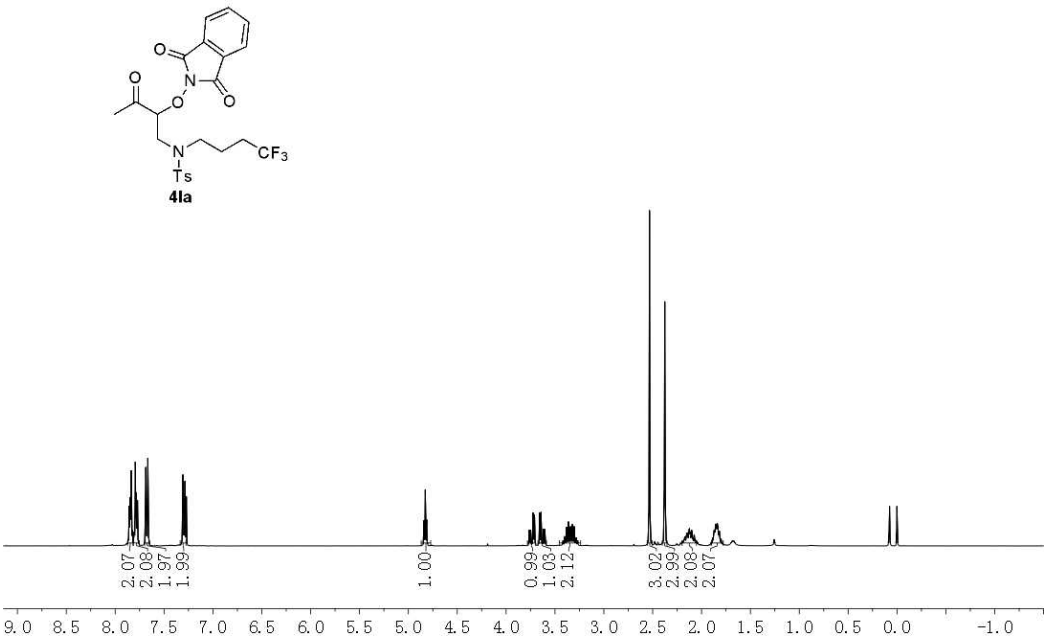
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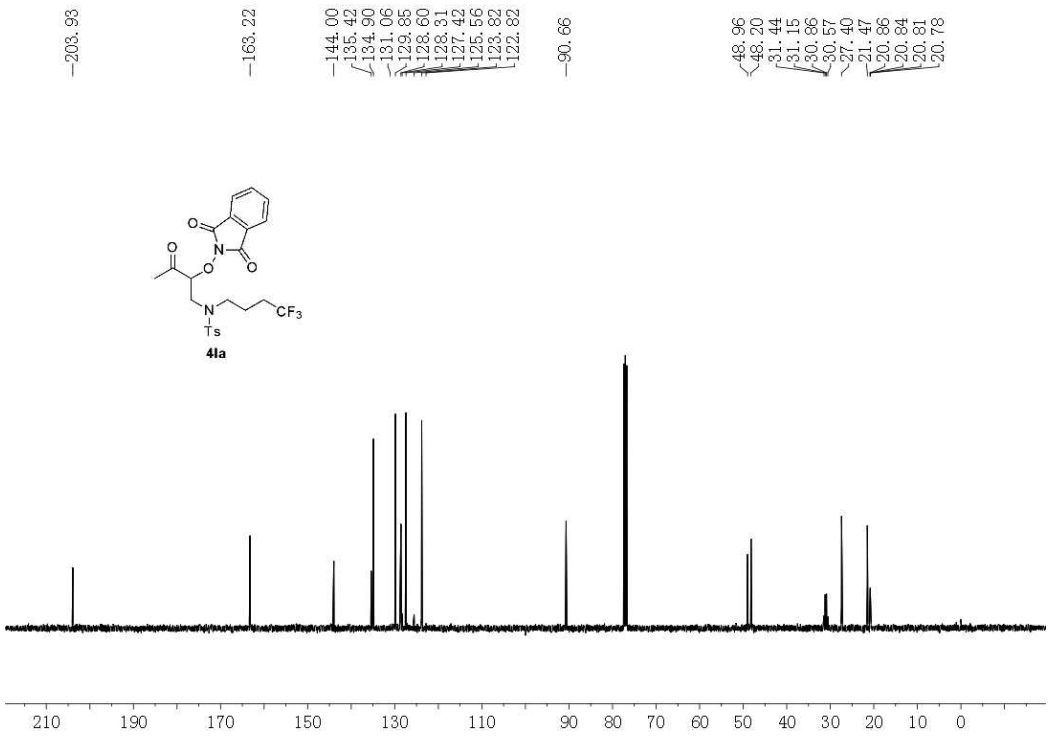
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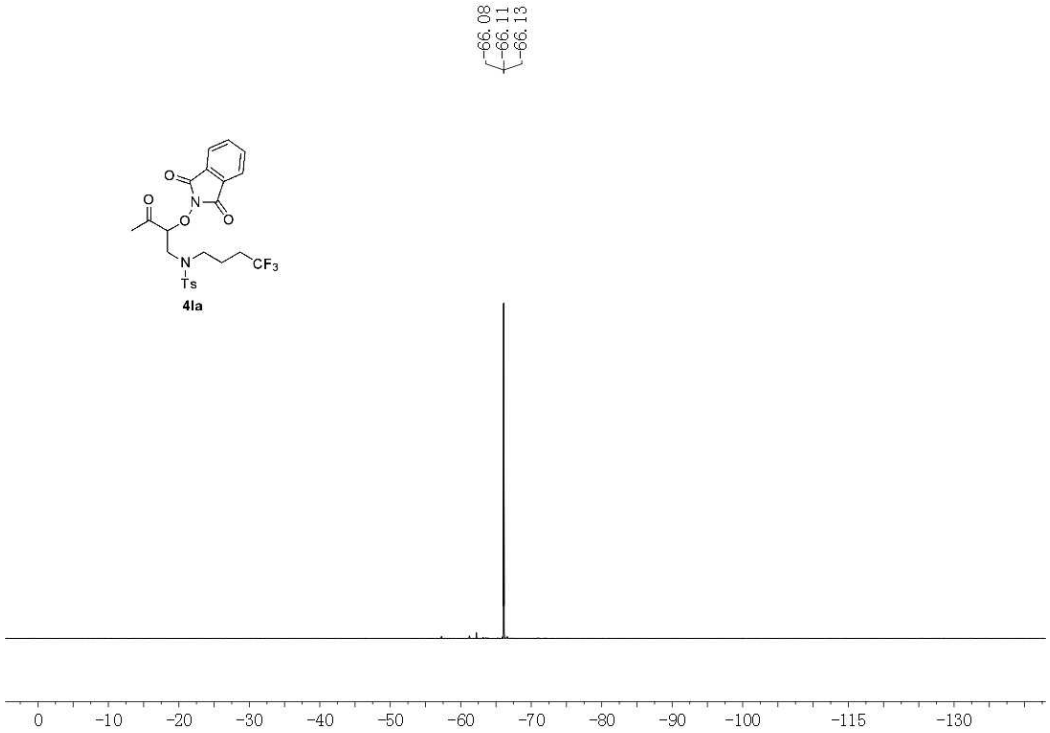
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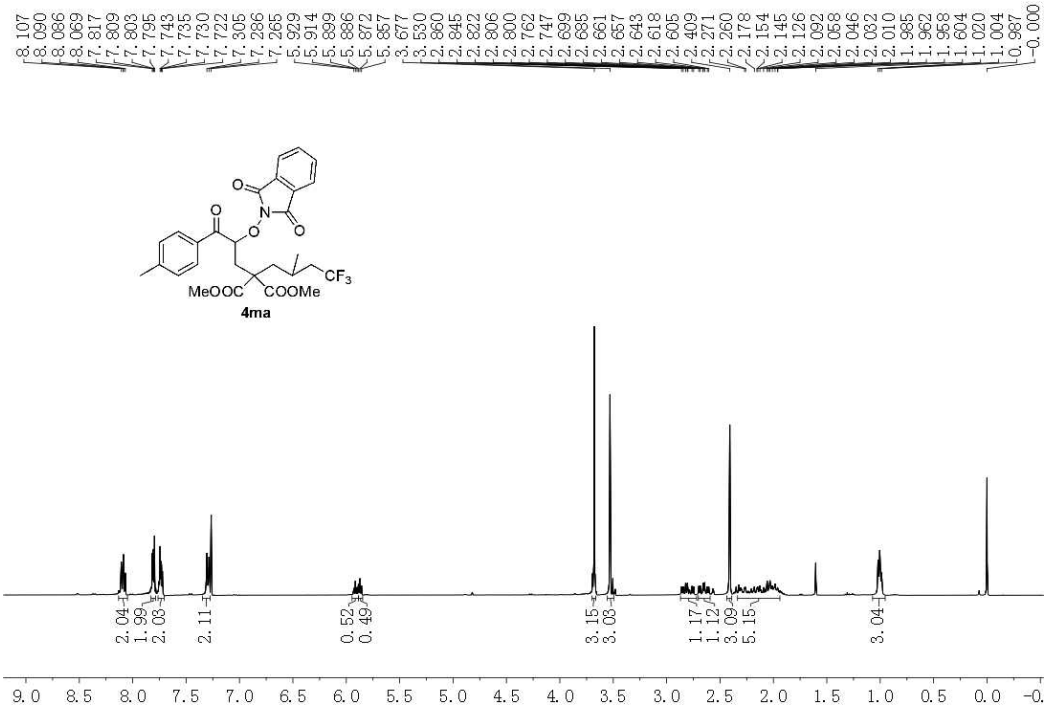
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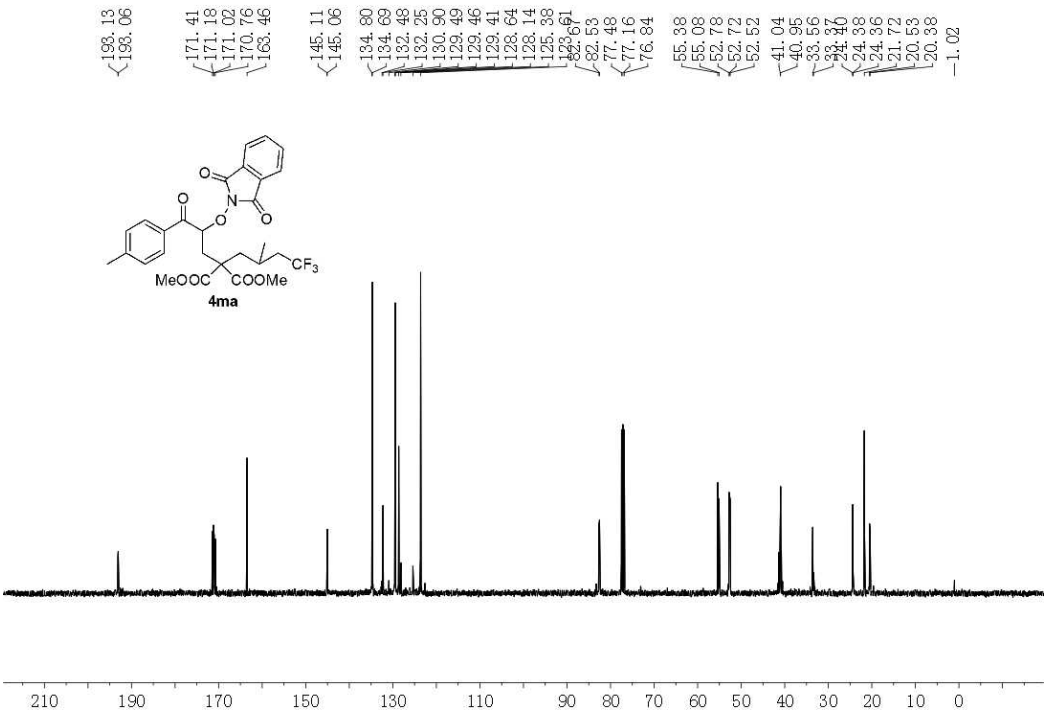
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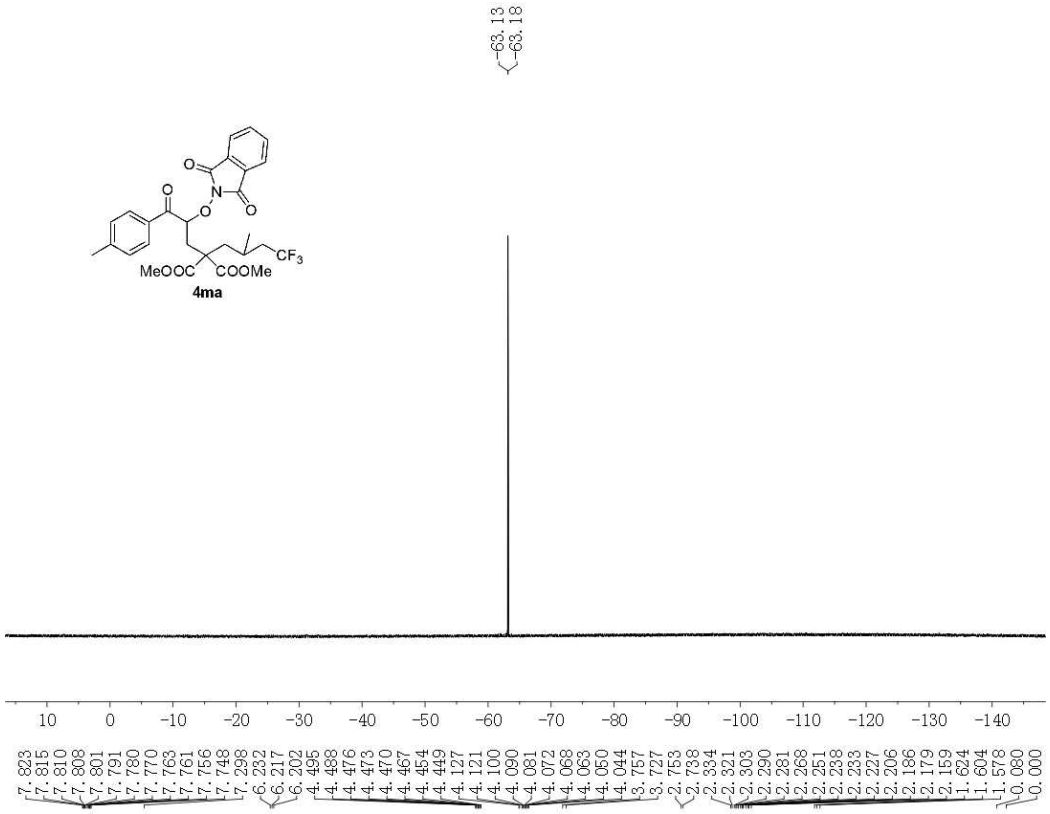
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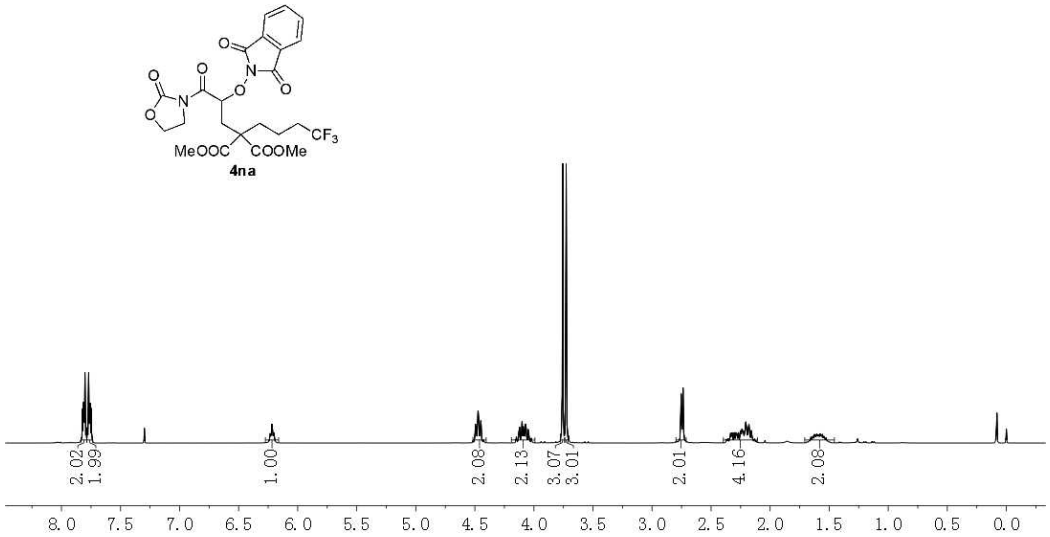
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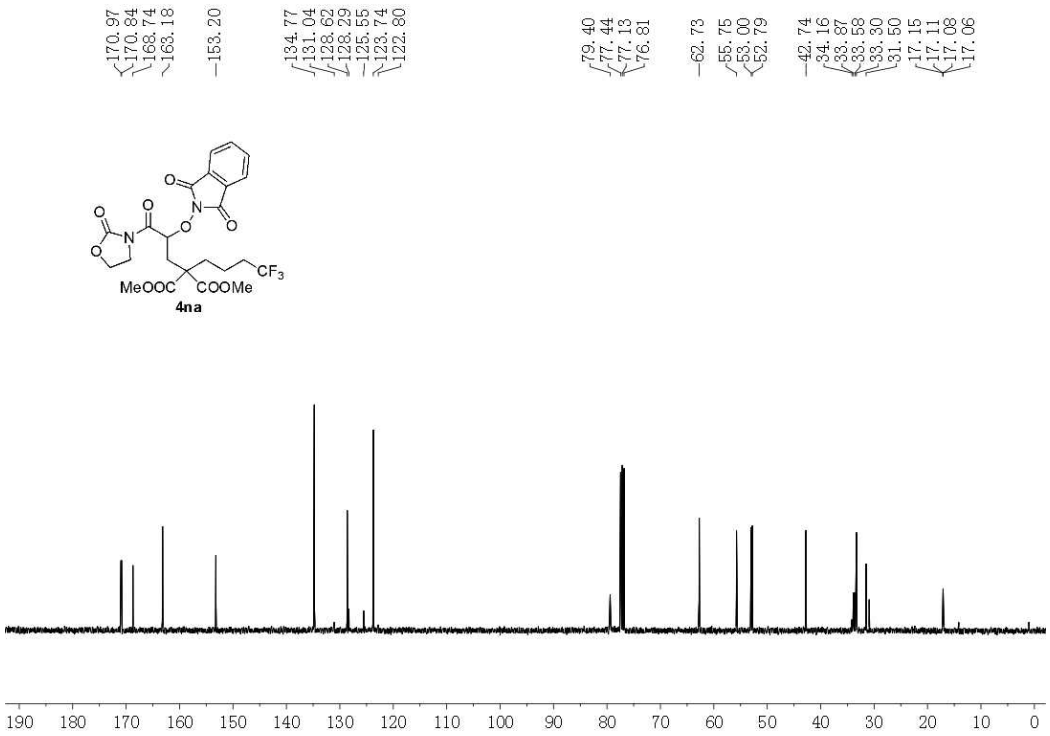
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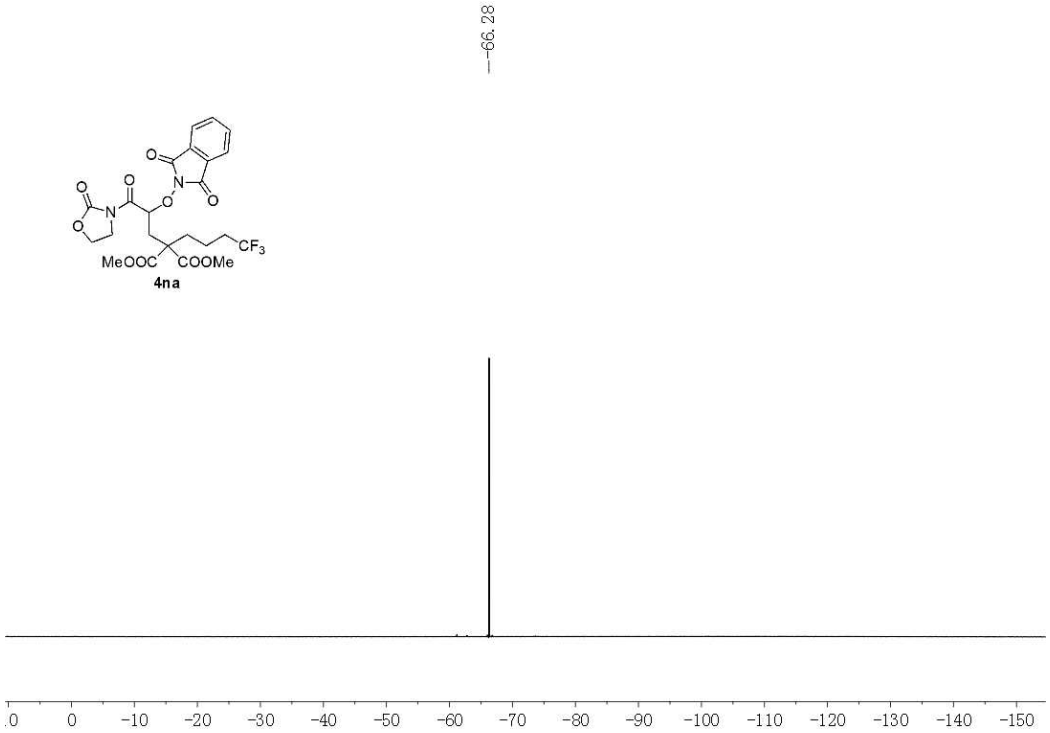
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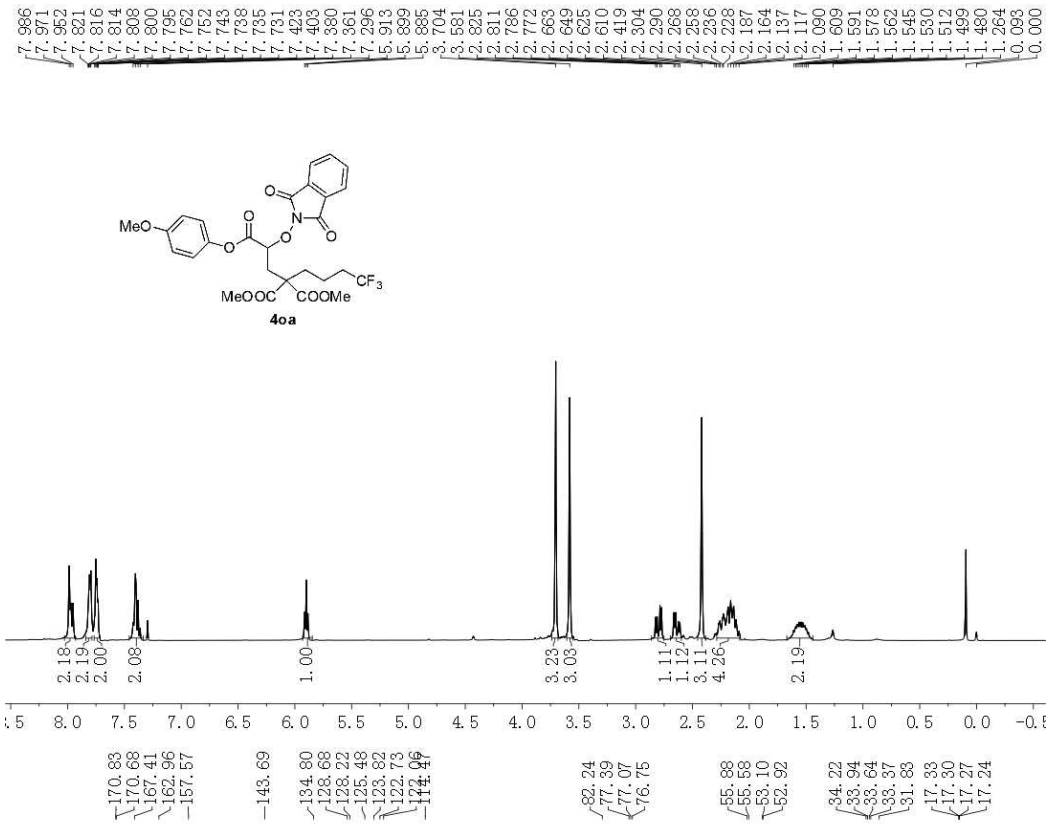
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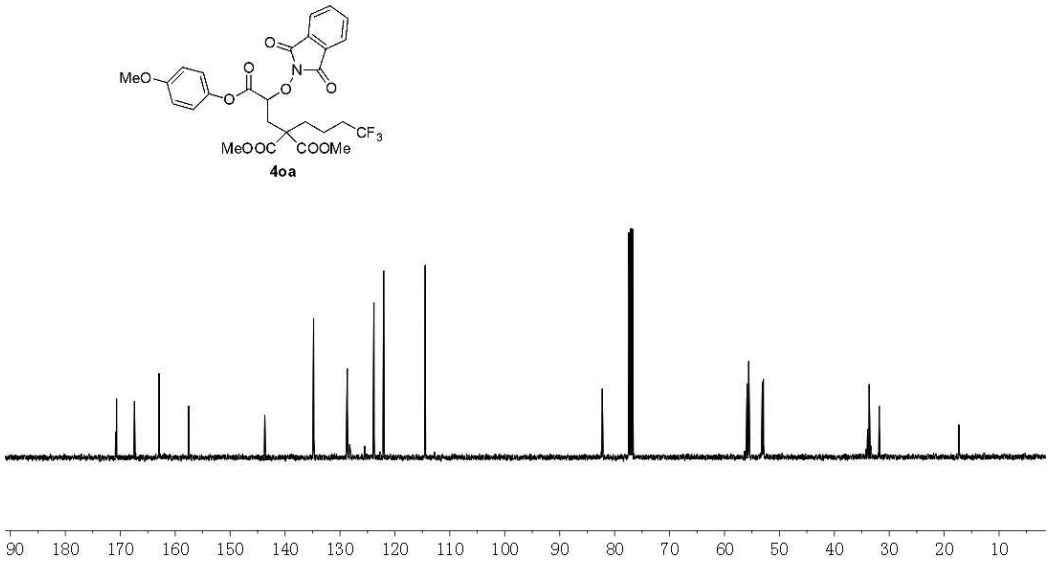
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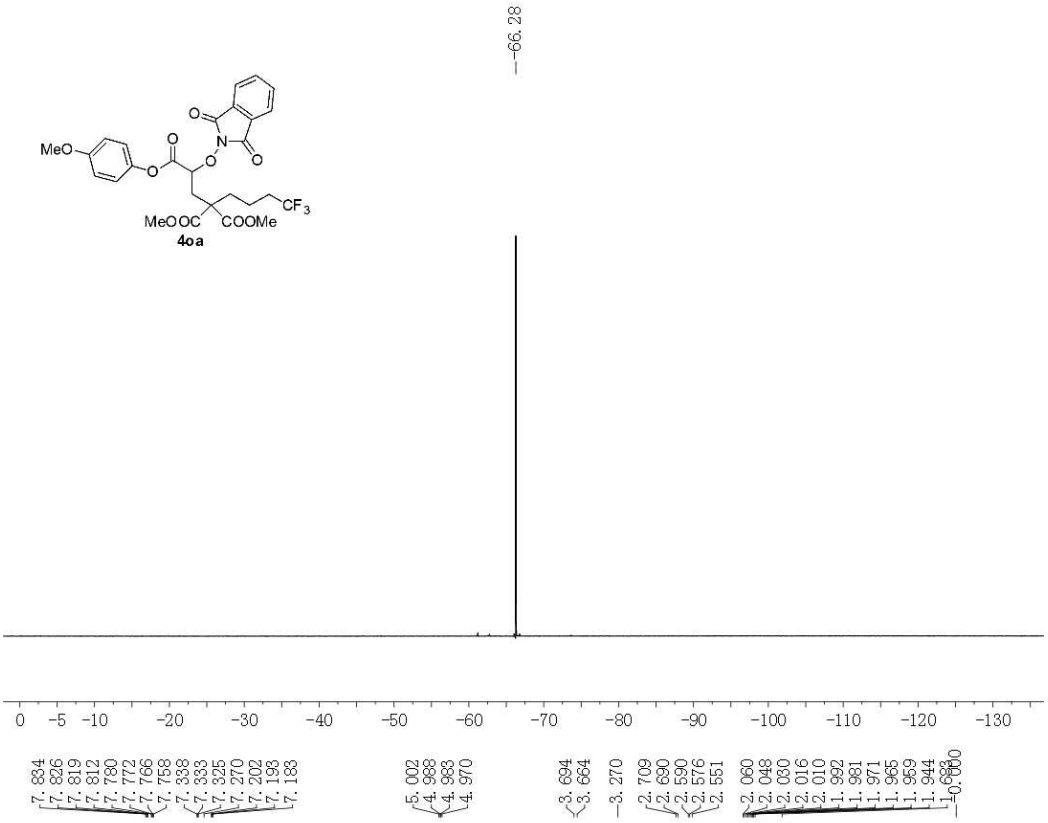
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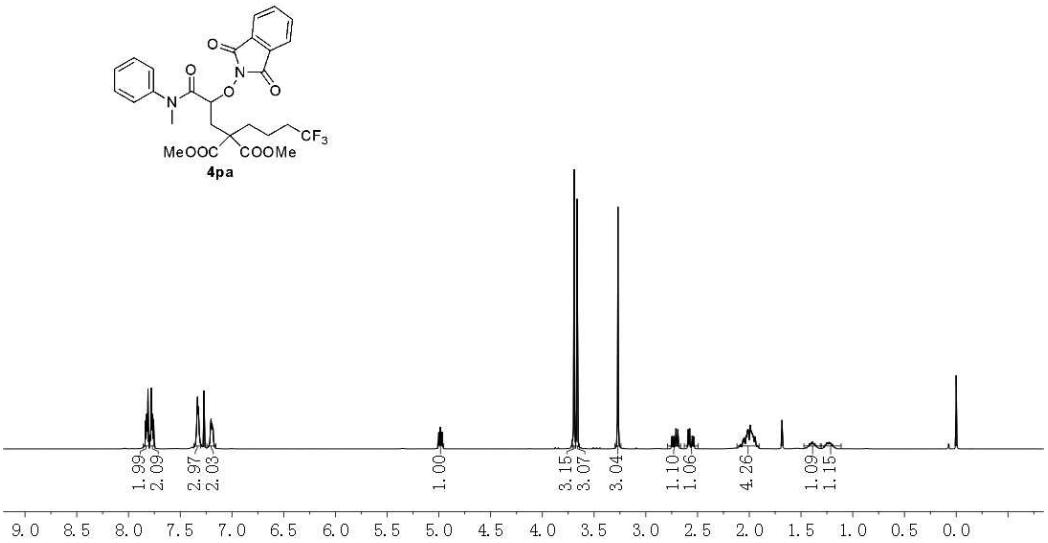
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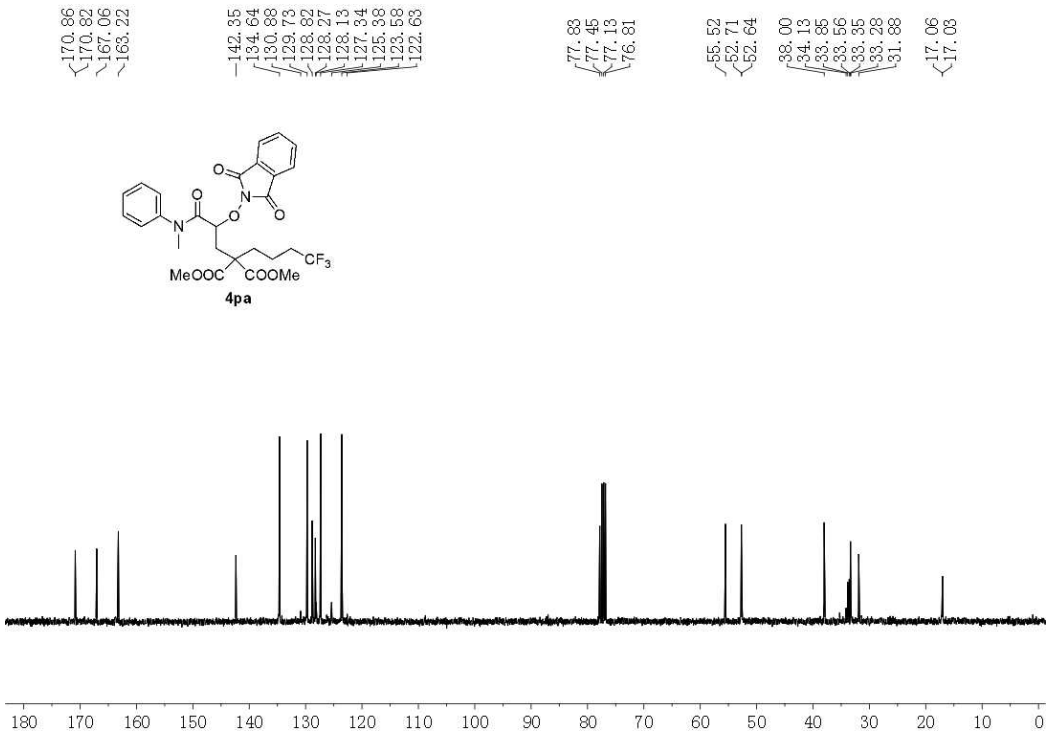
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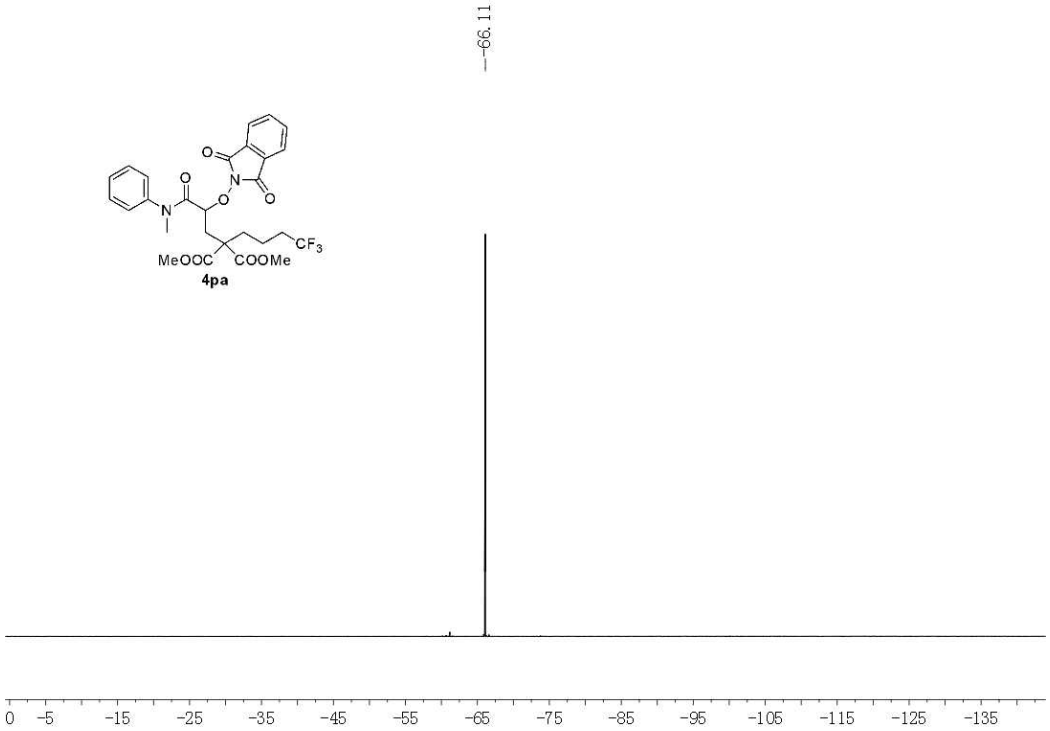
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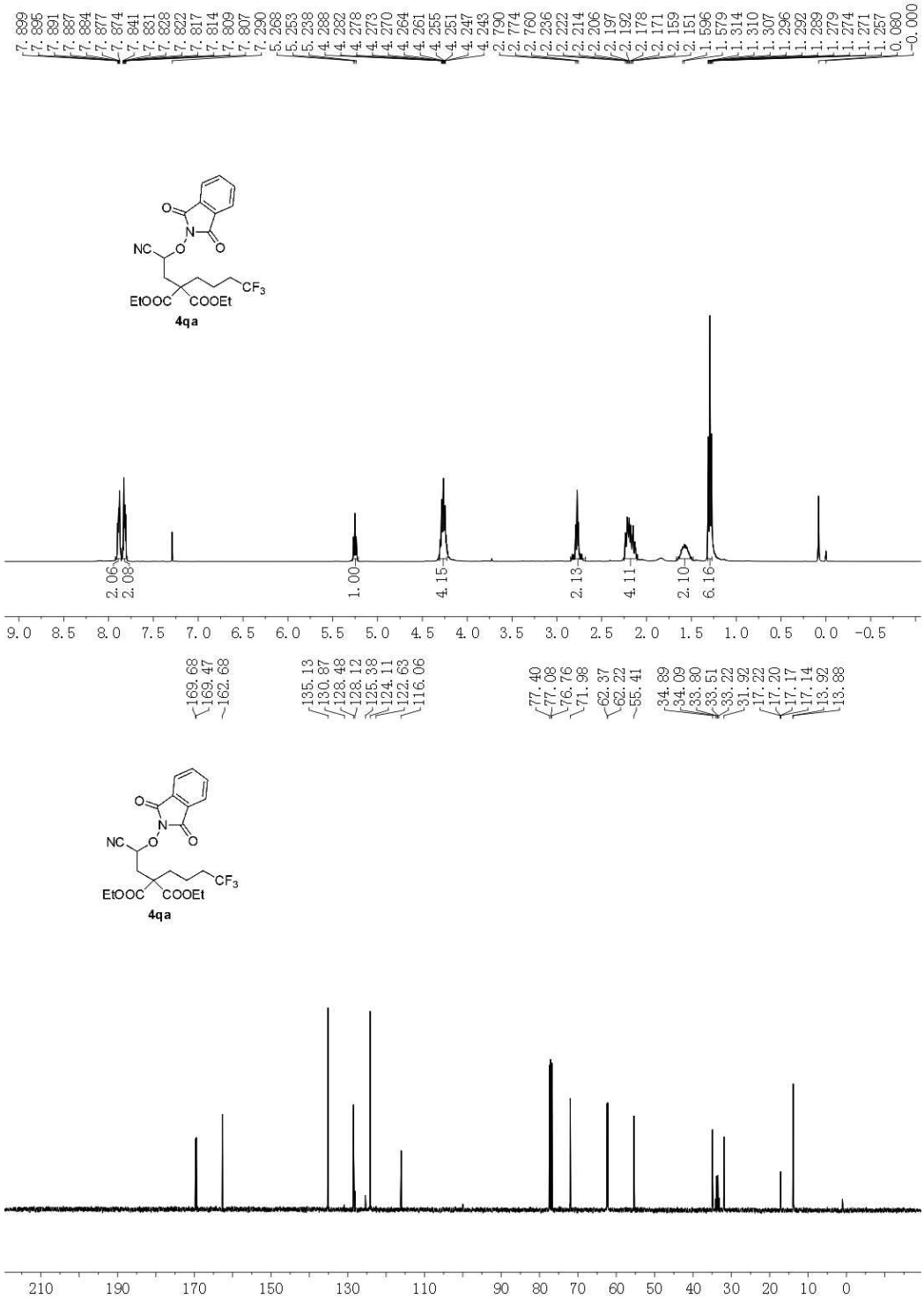
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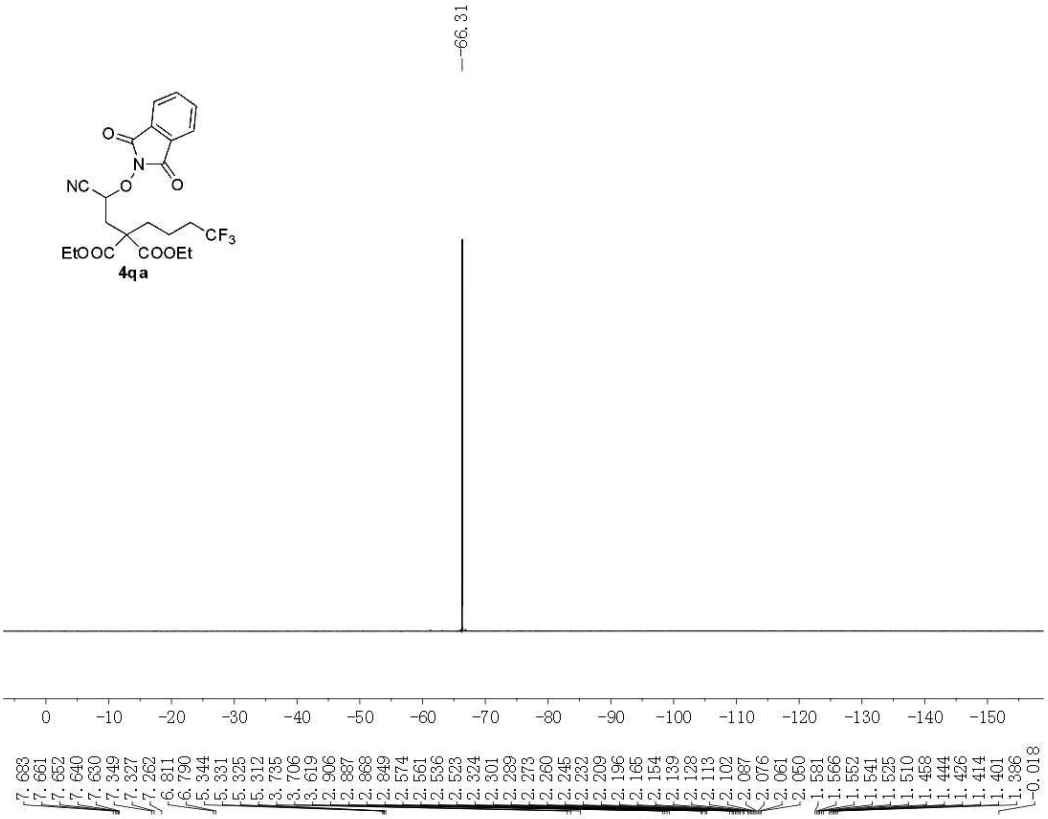
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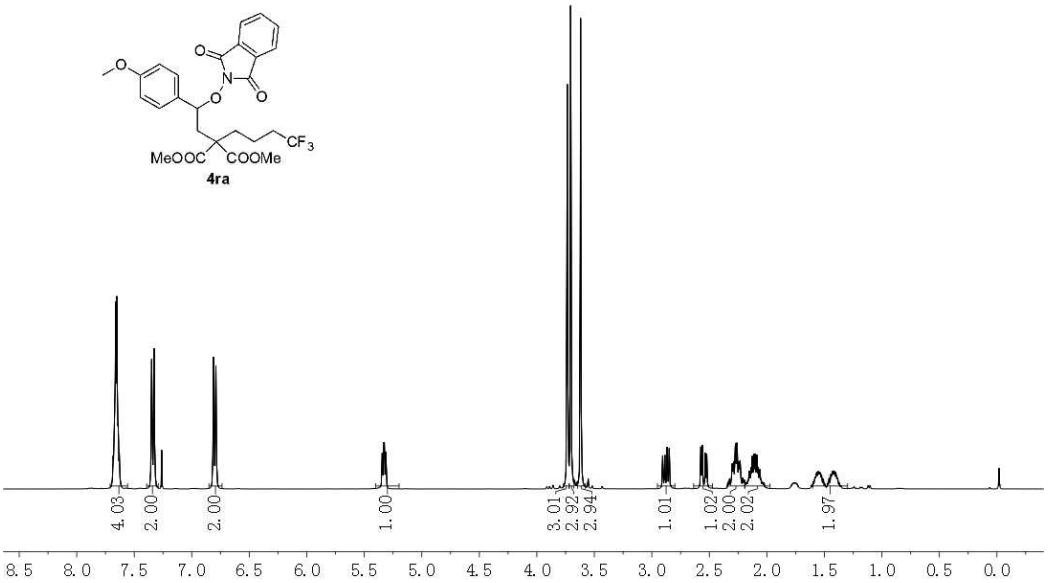
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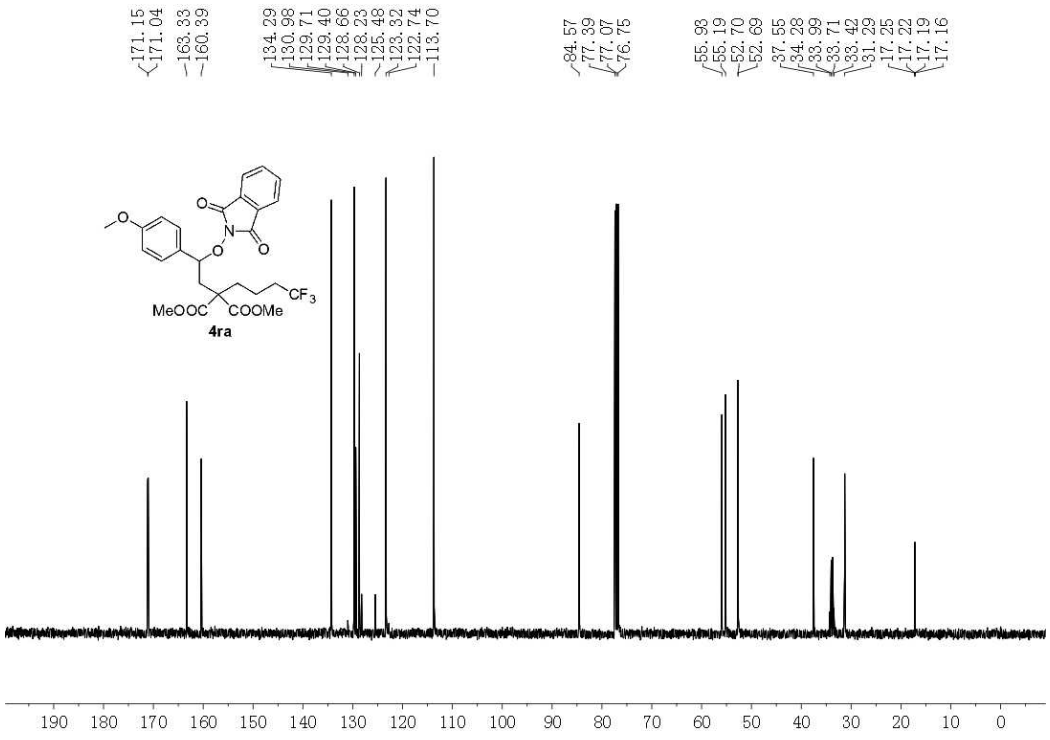
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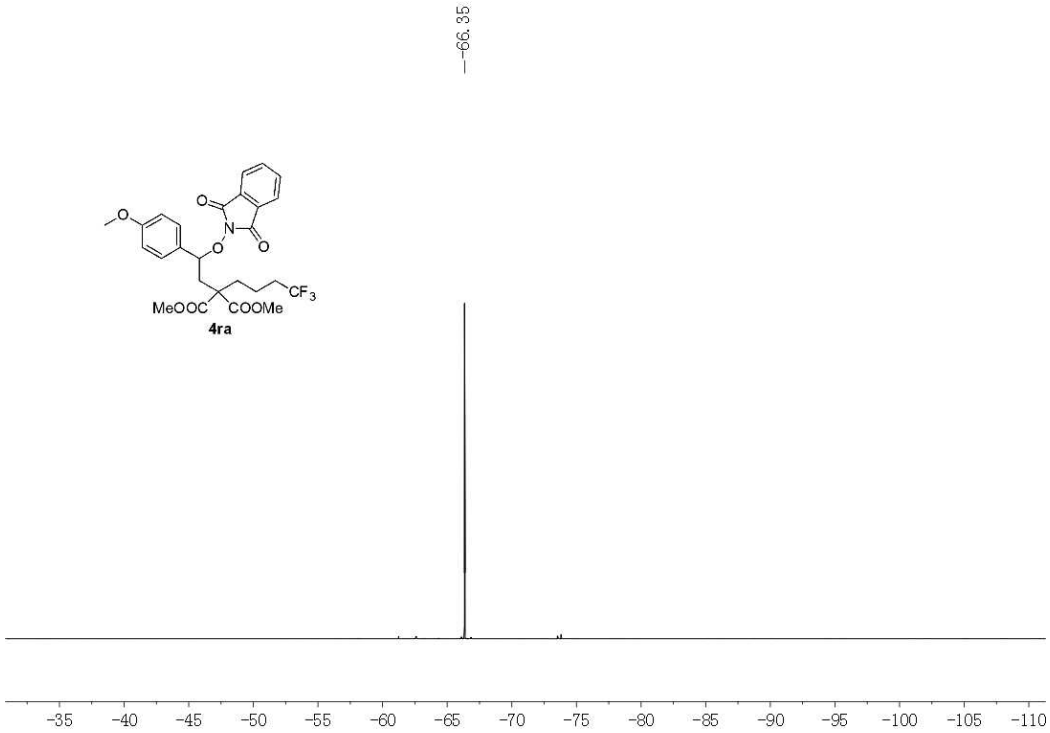
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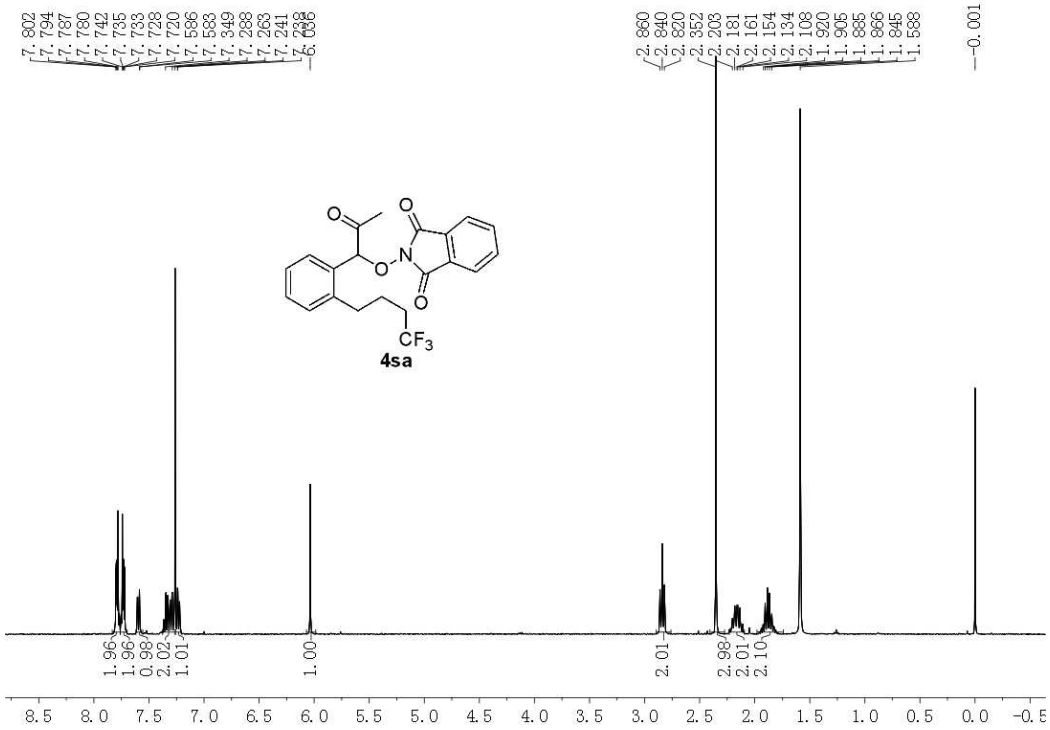
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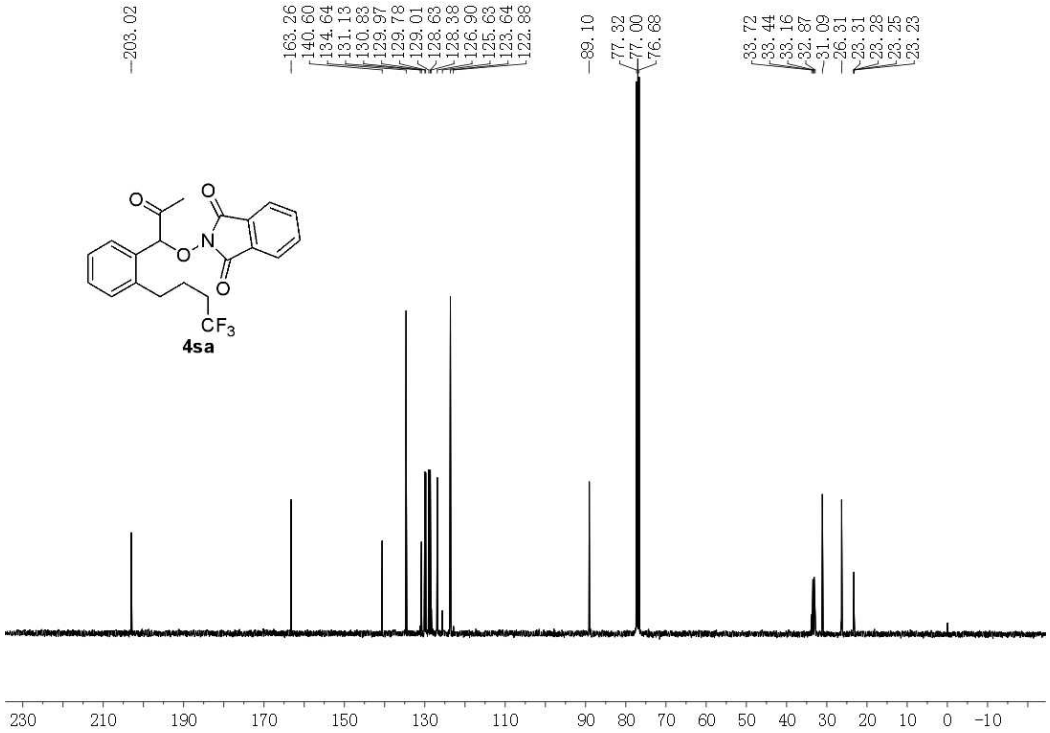
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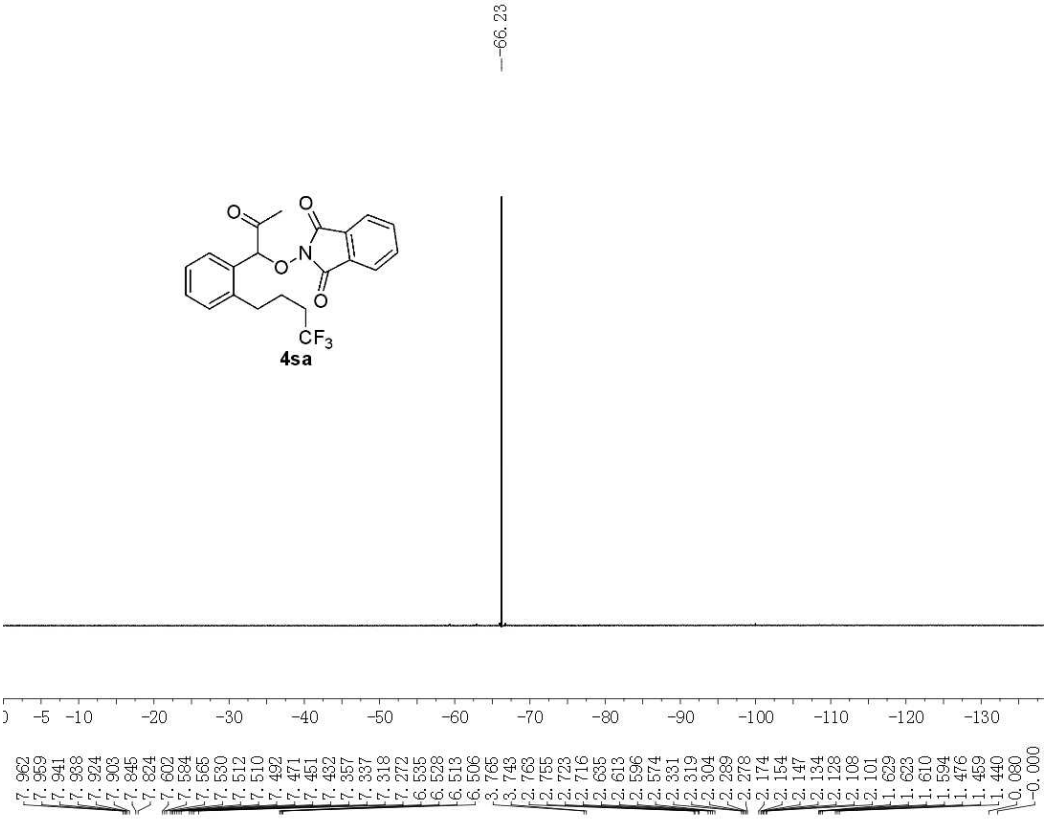
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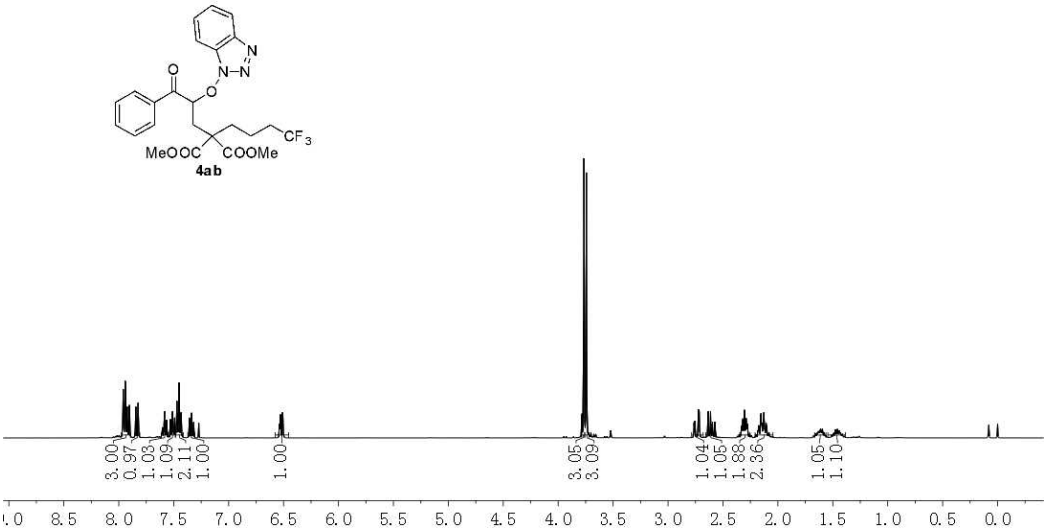
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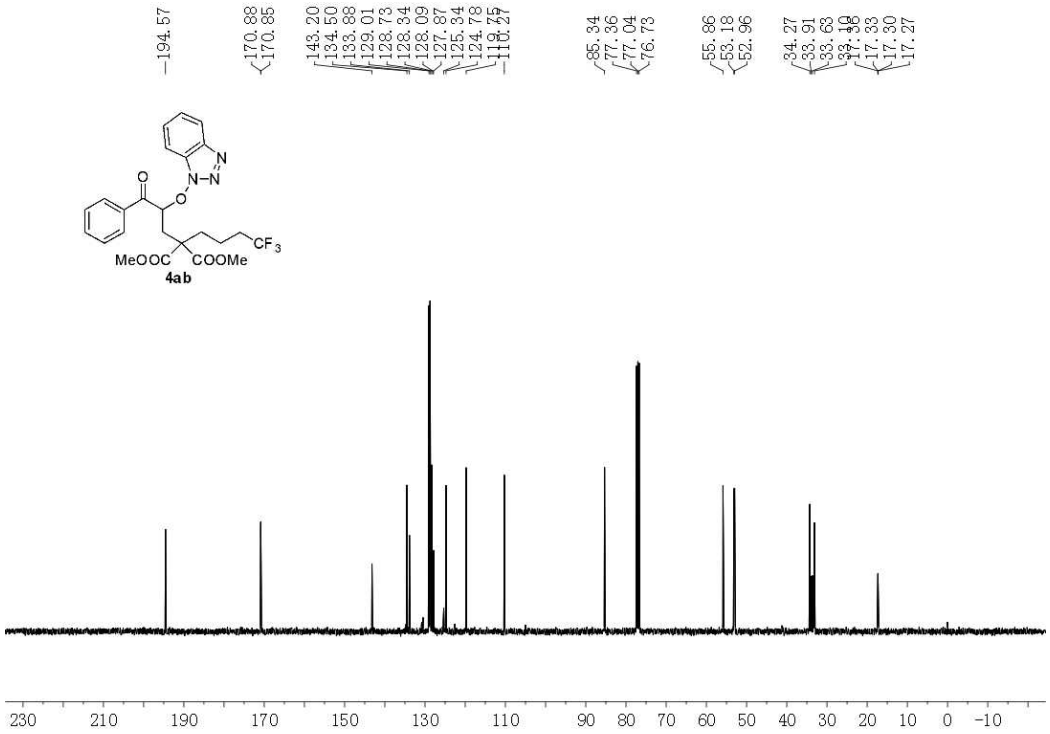
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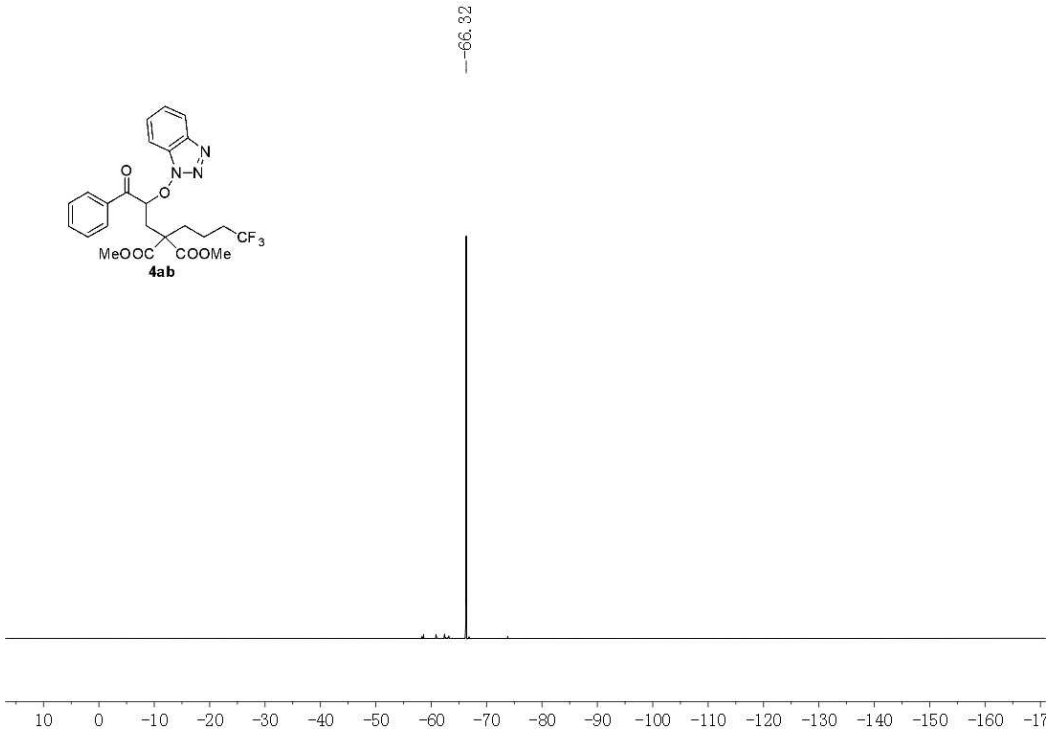
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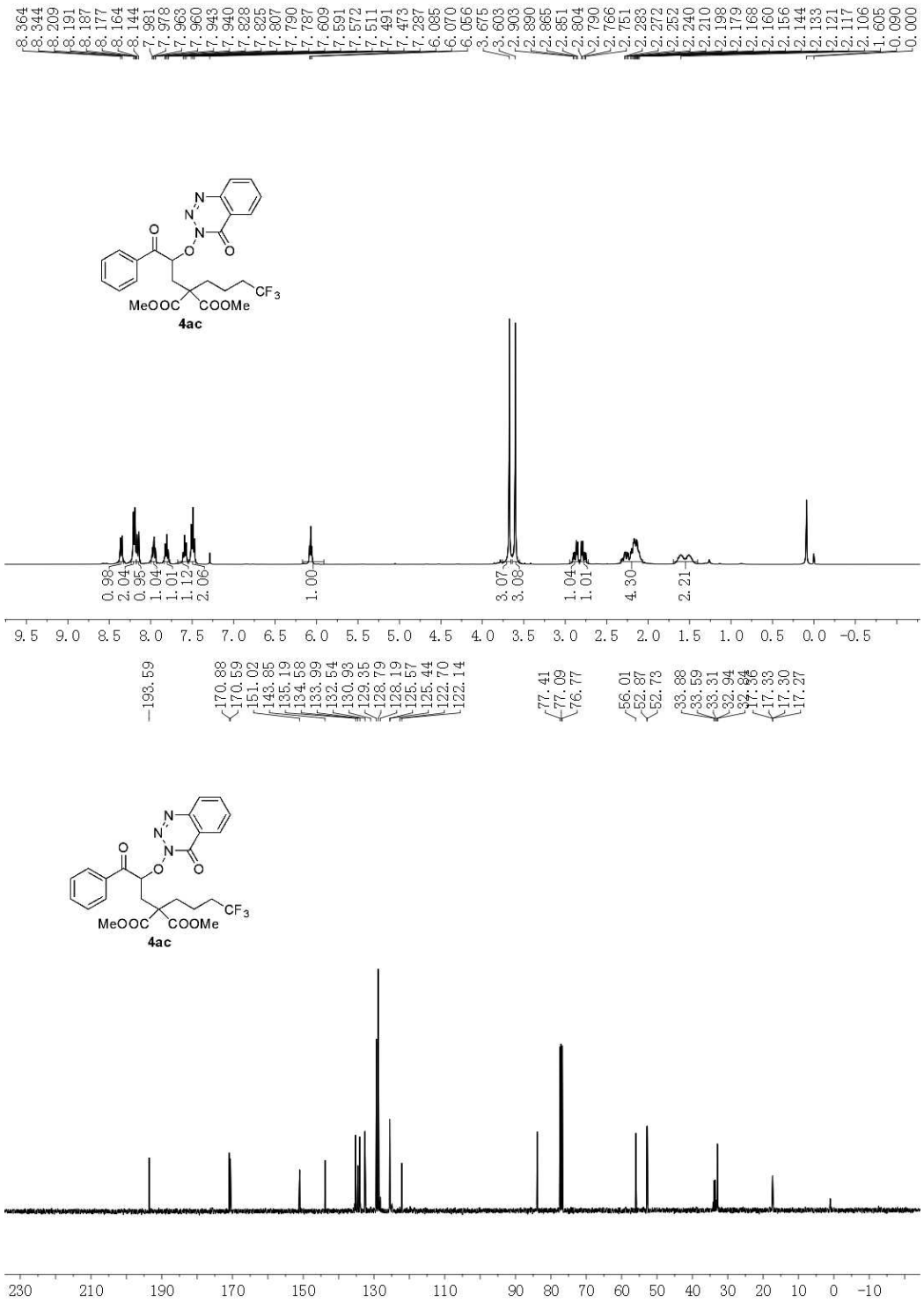
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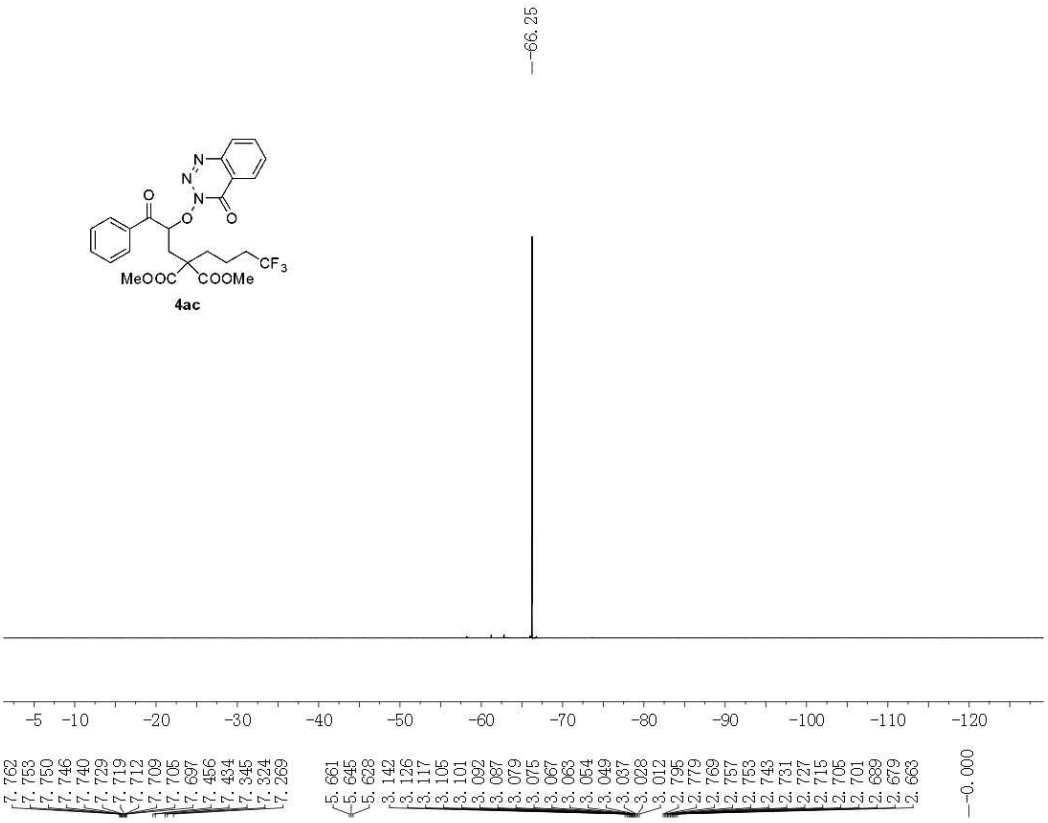
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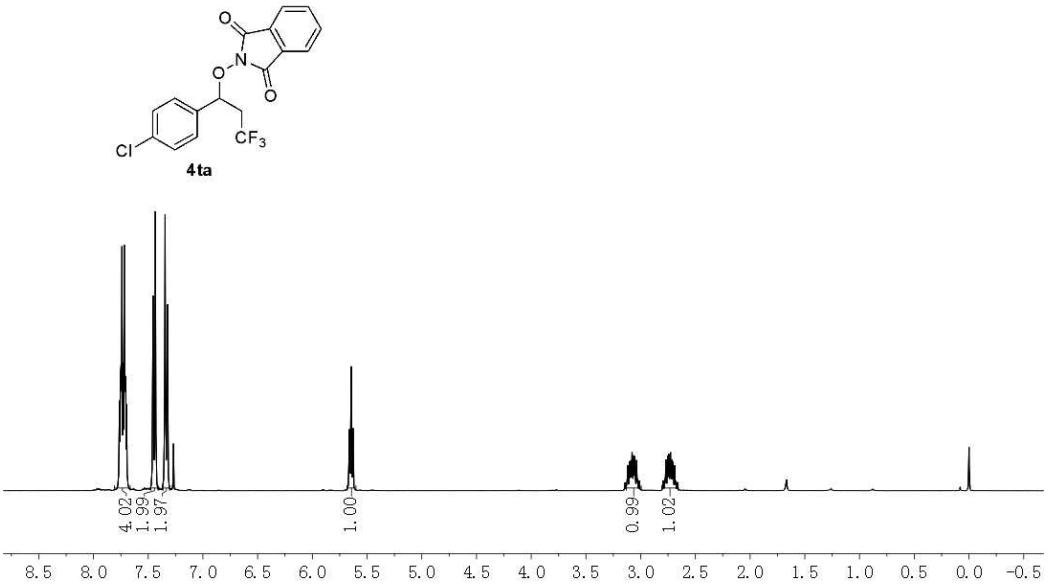
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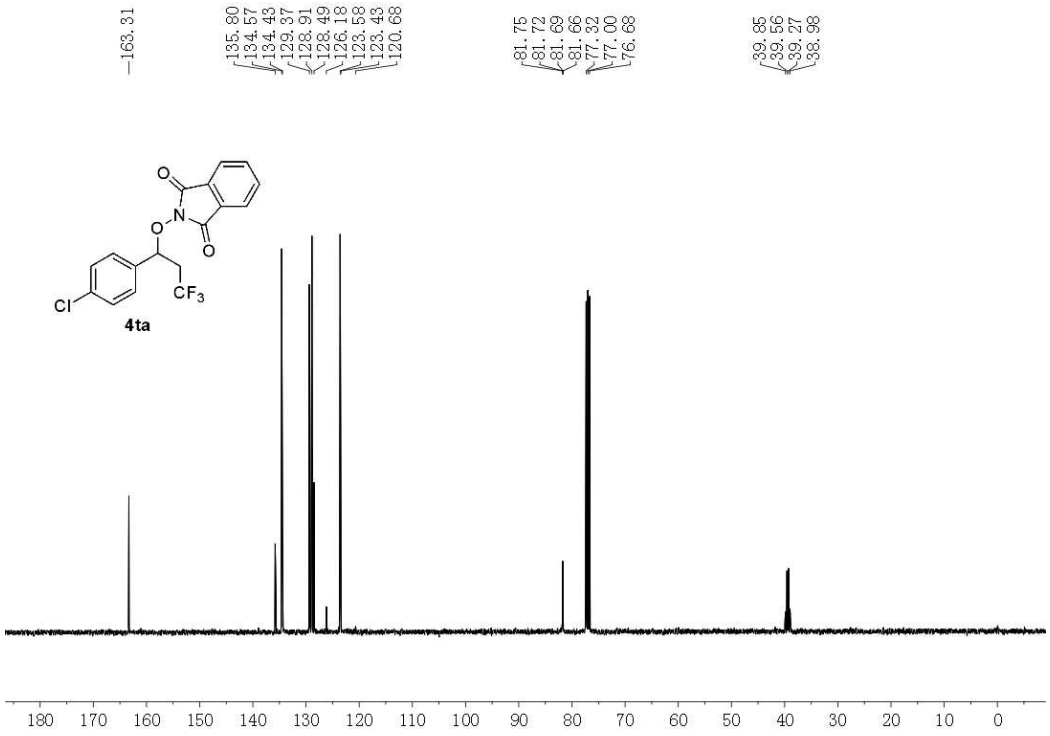
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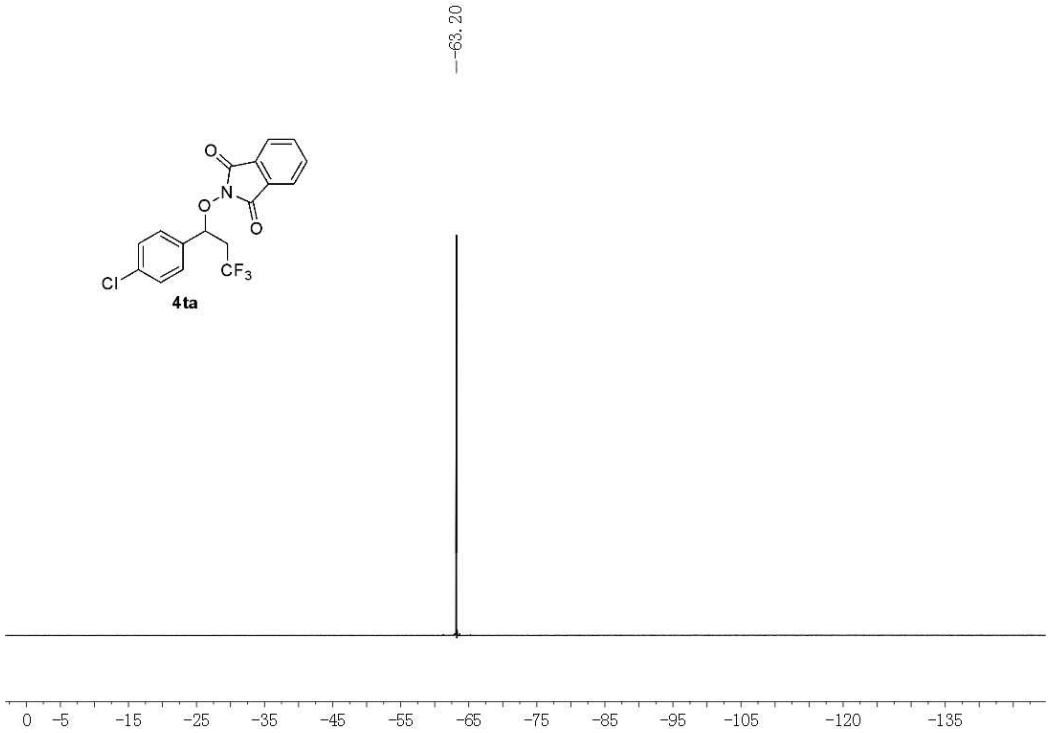
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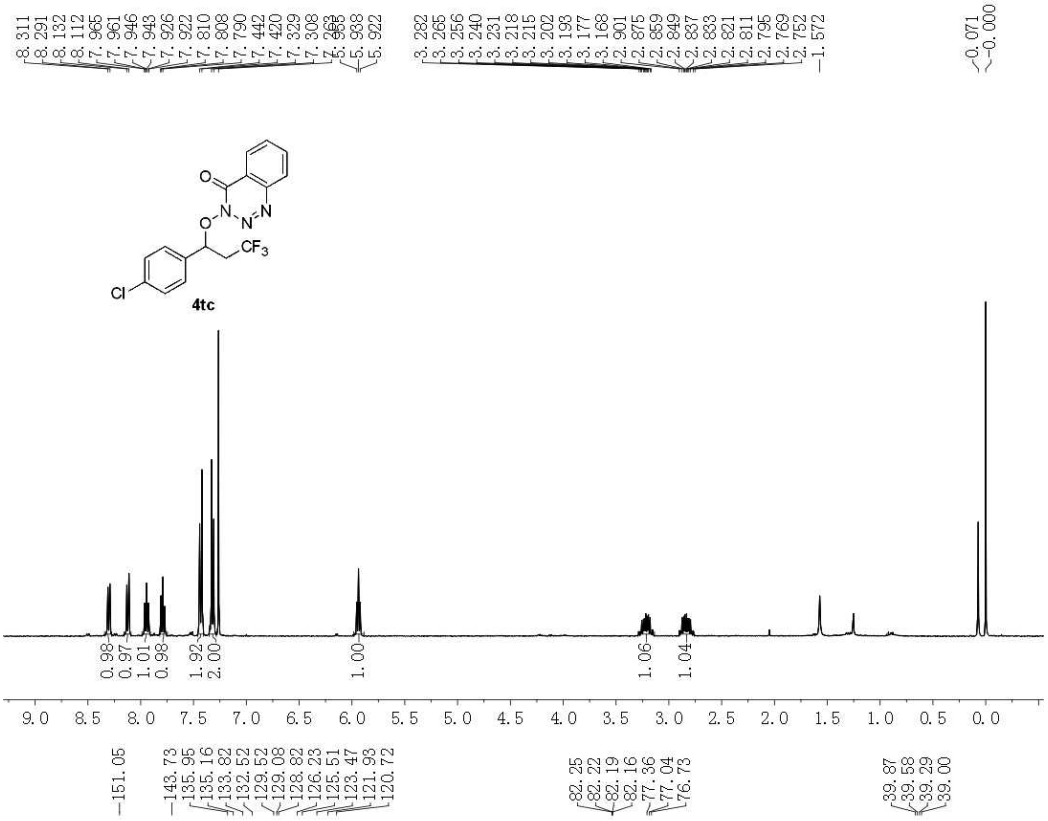
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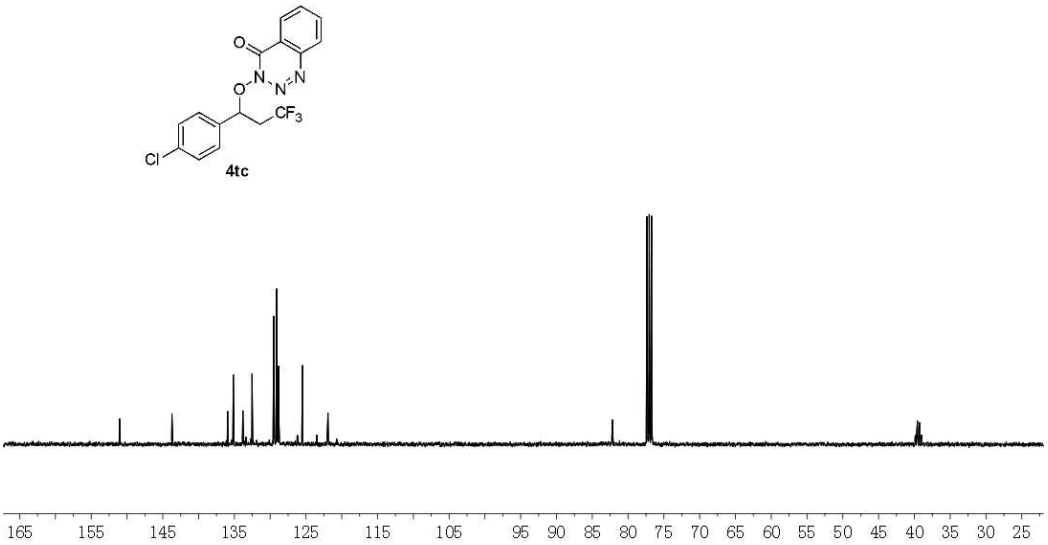
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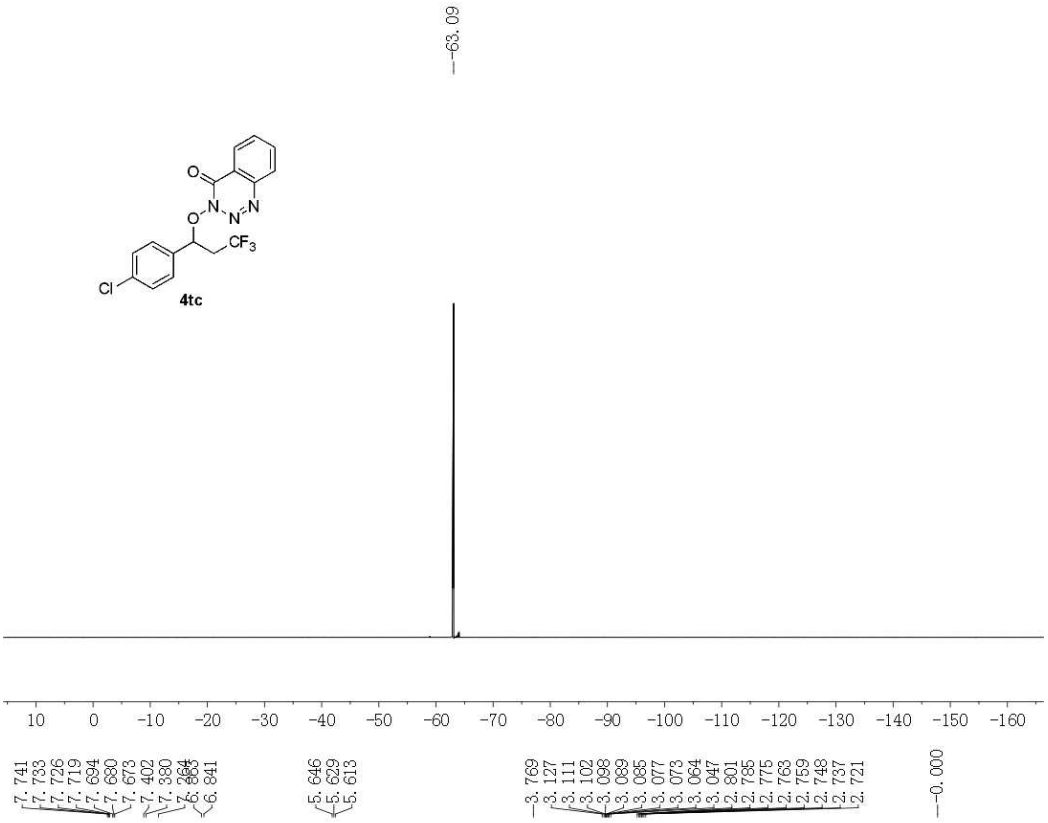
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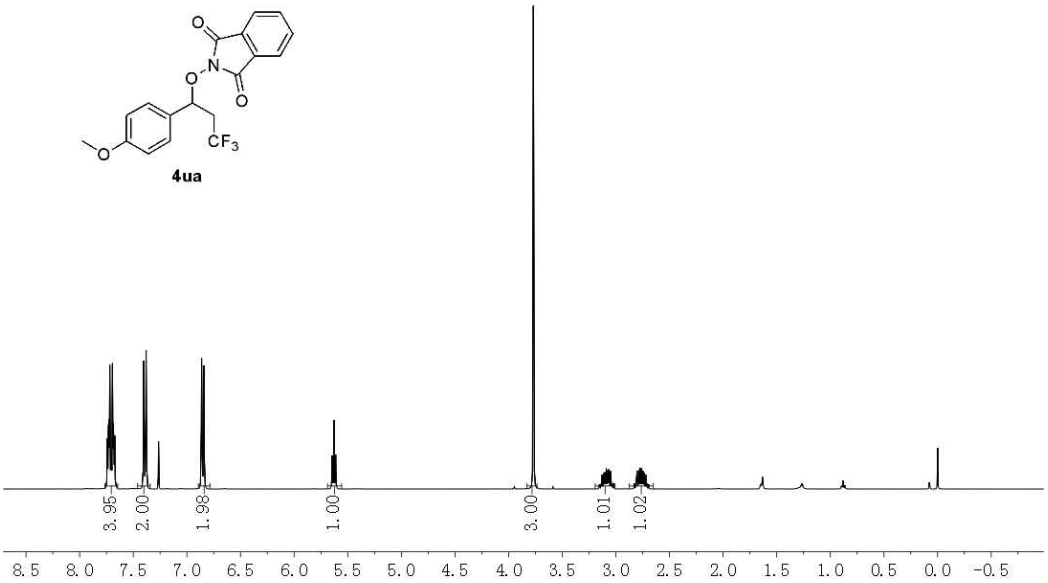
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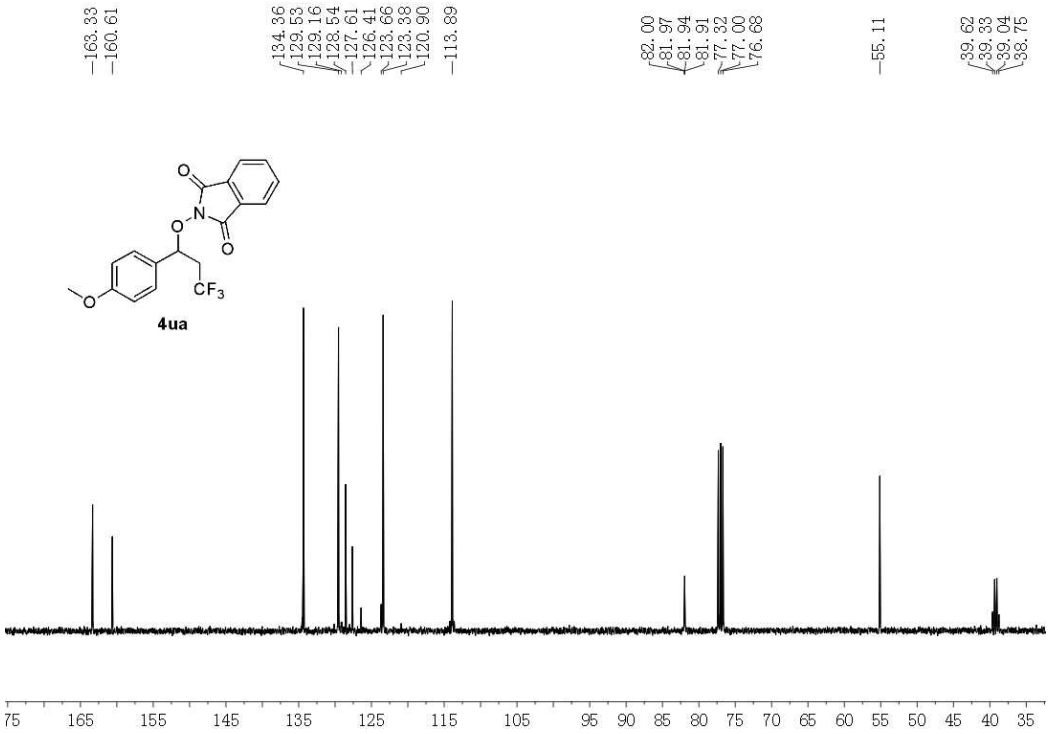
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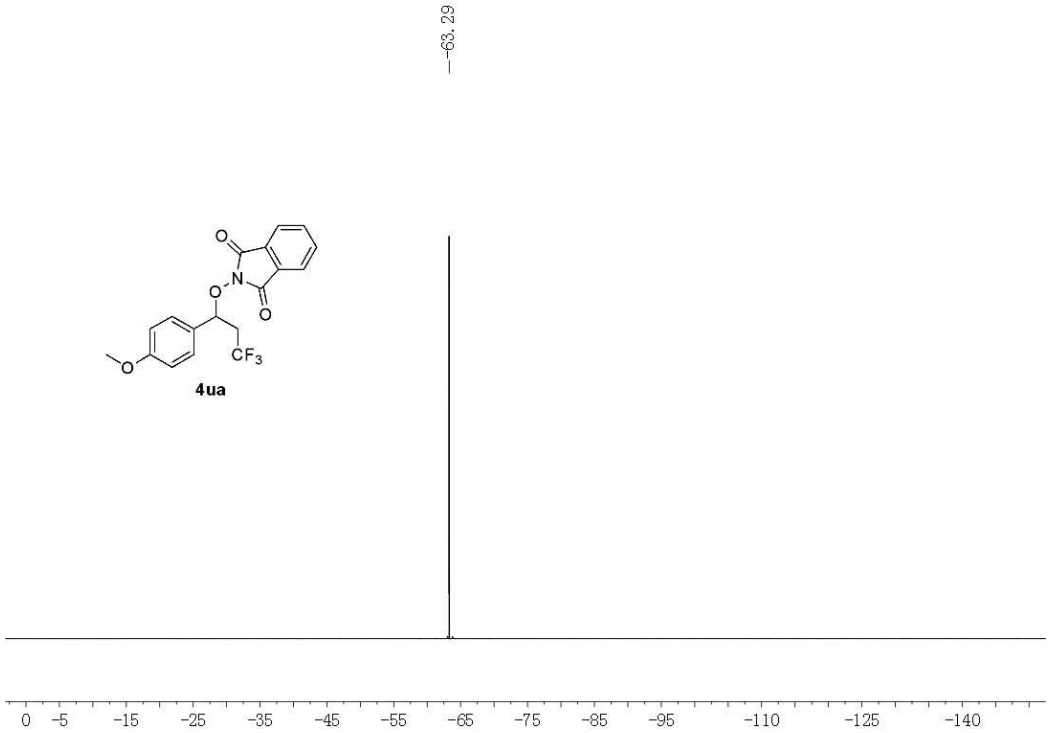
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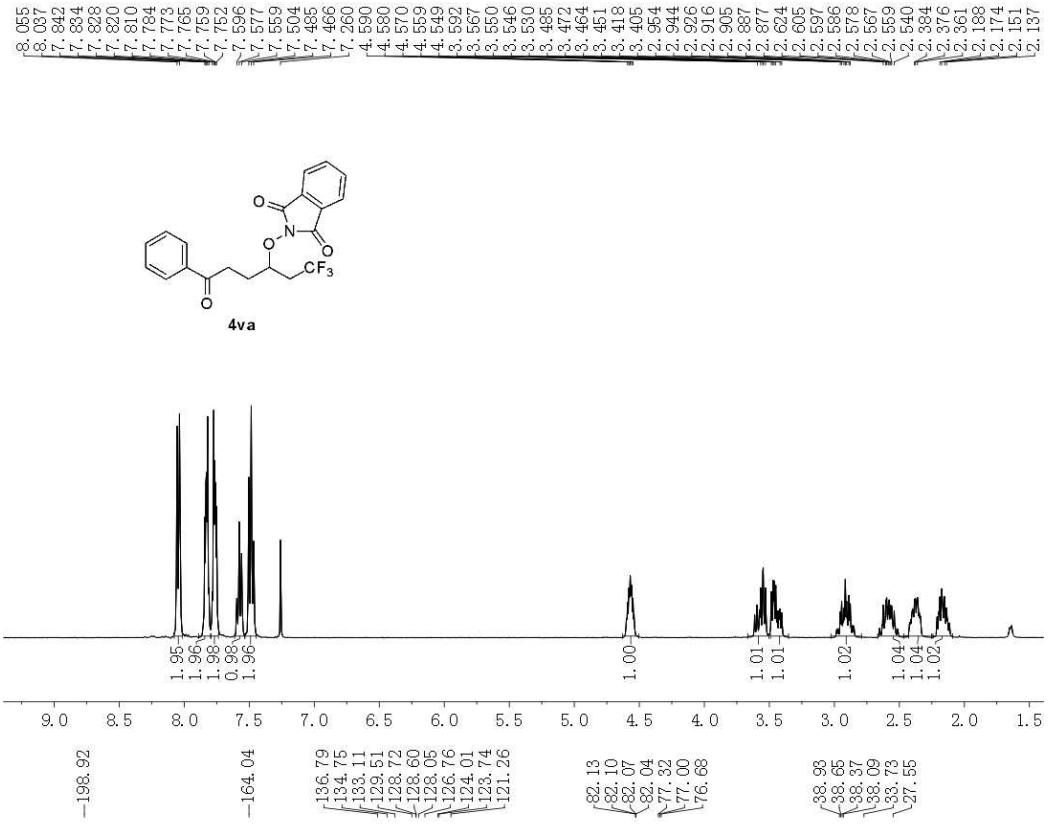
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1.01
1.01
1.02
1.04
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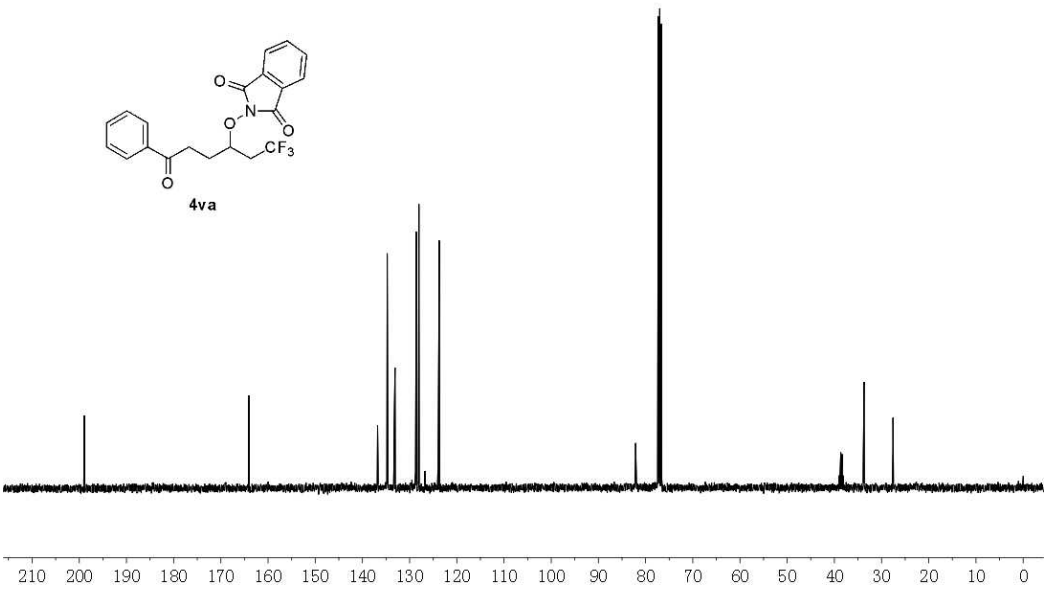
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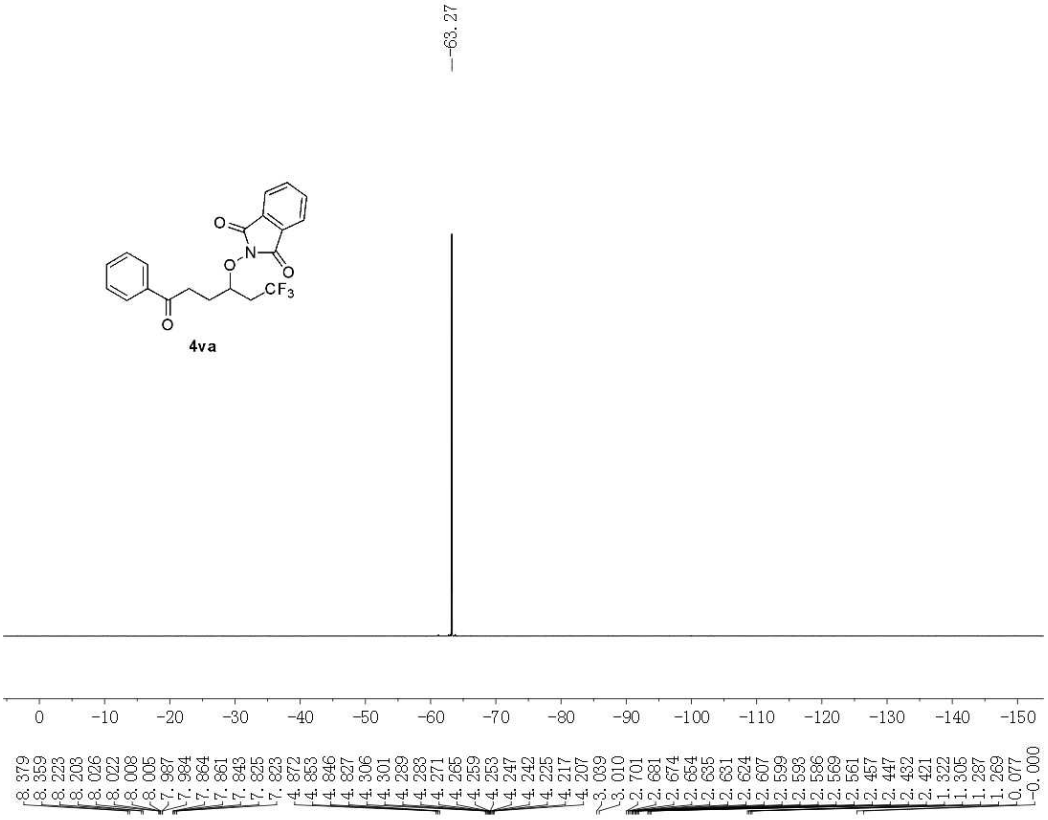
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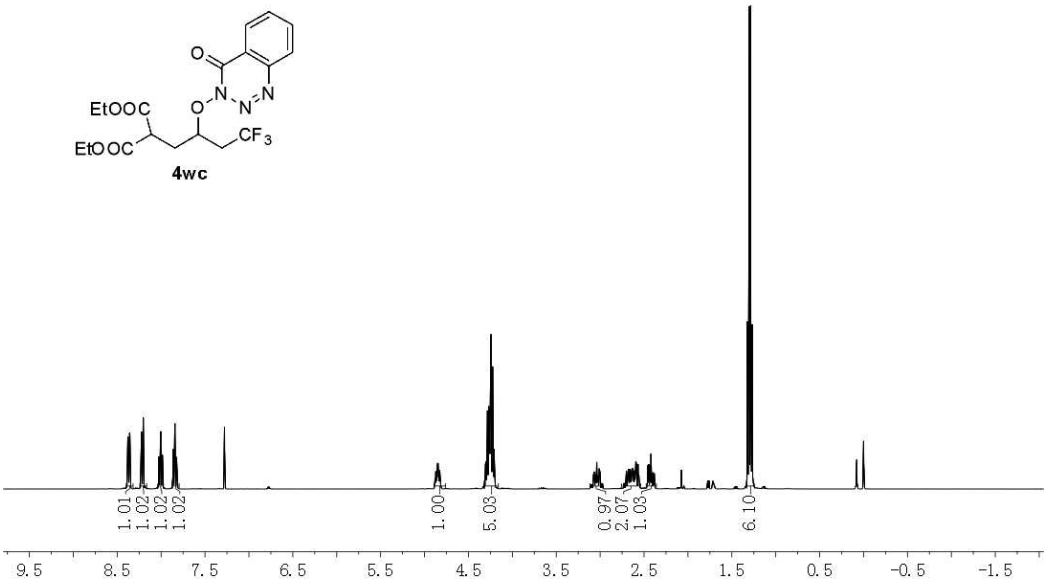
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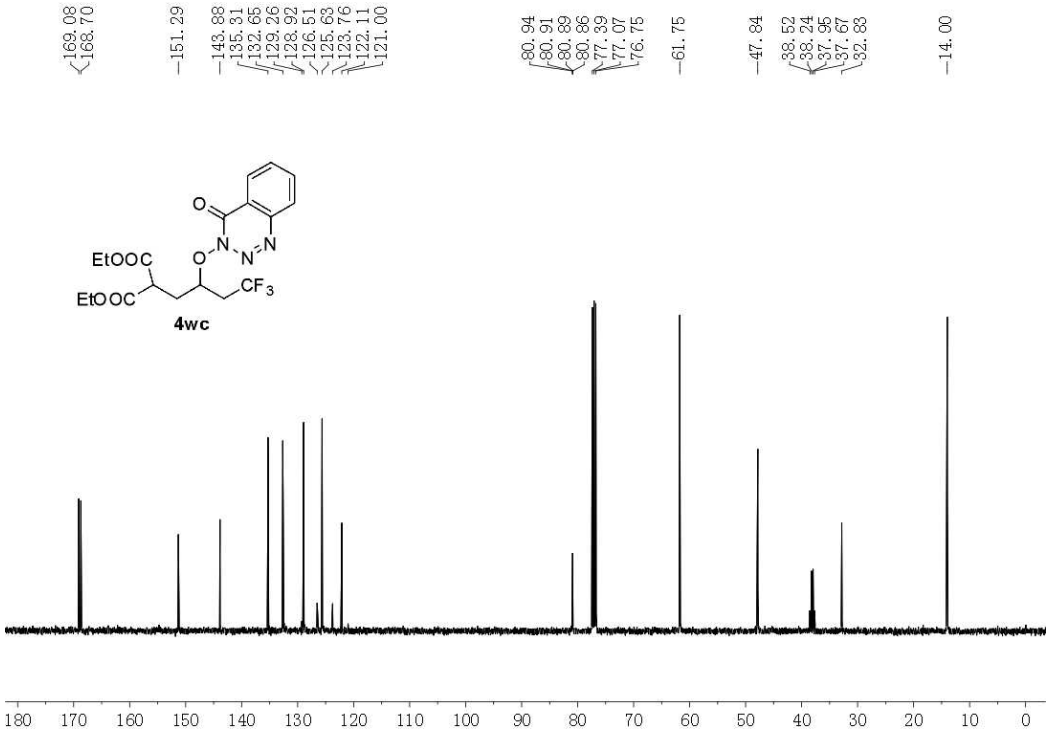
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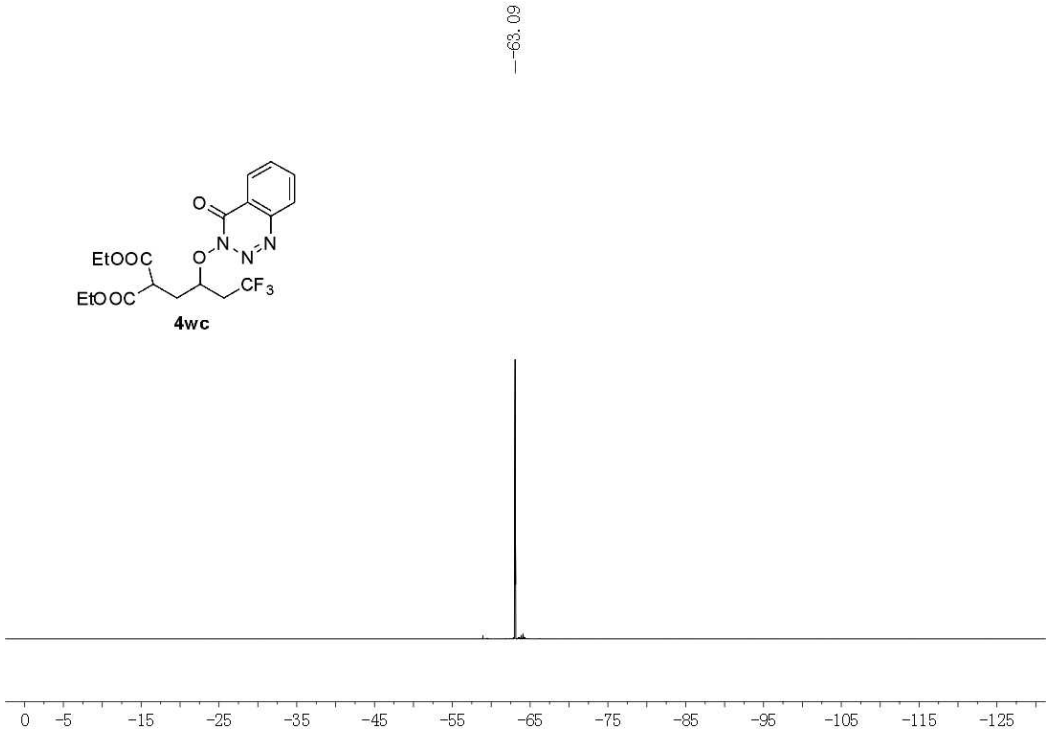
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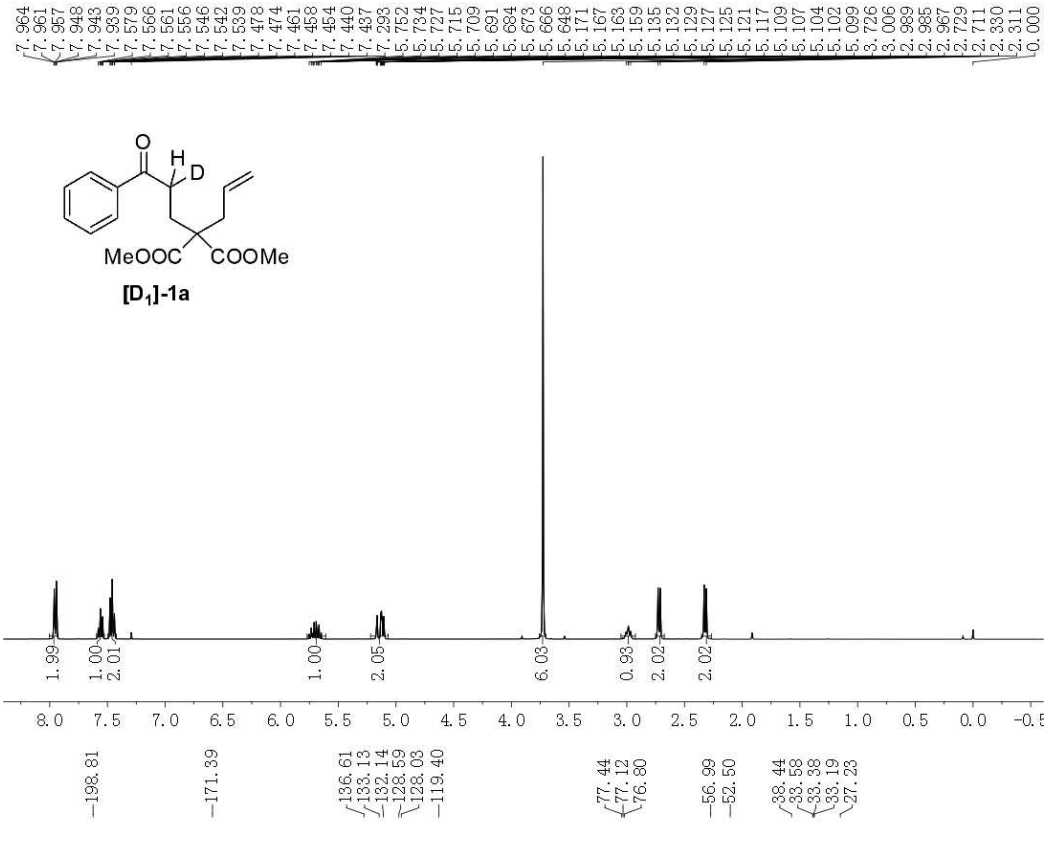
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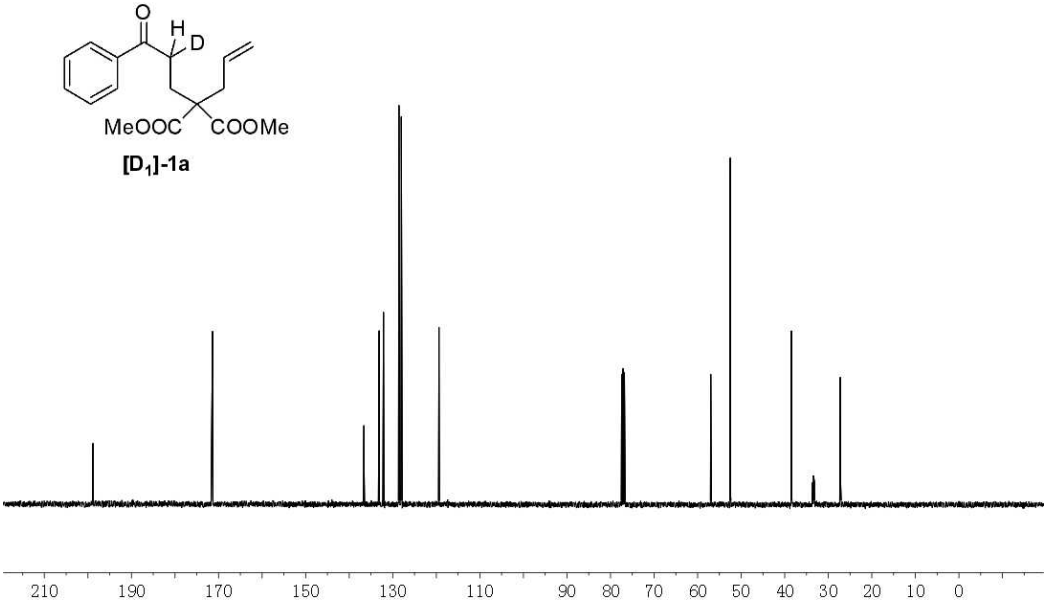
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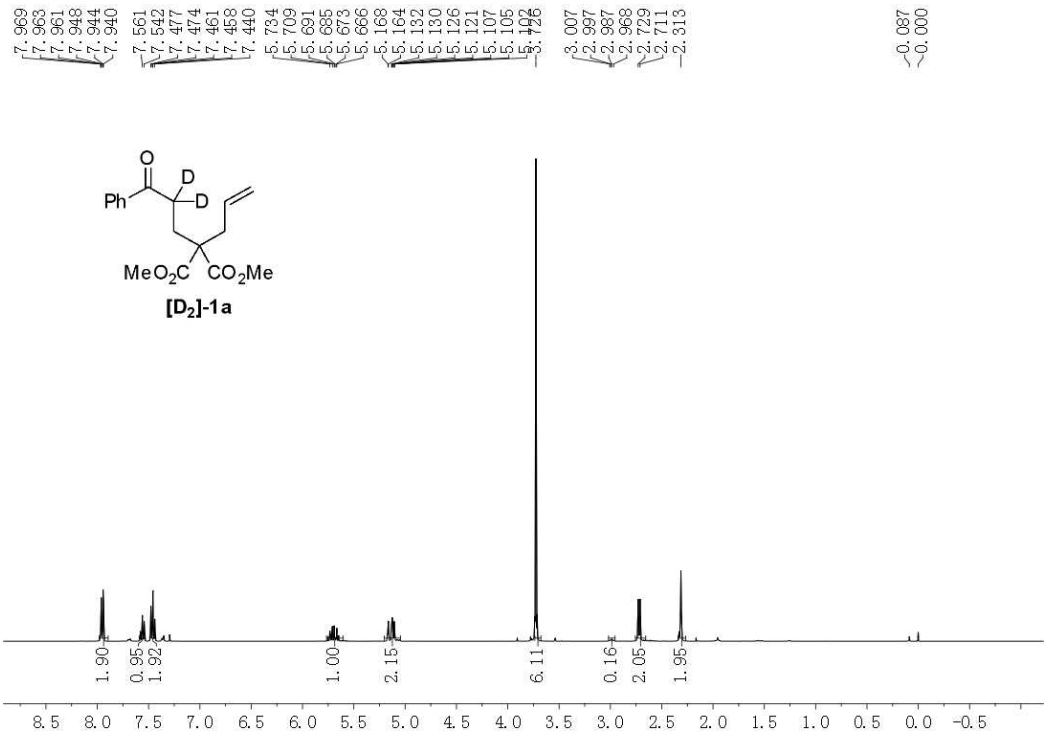
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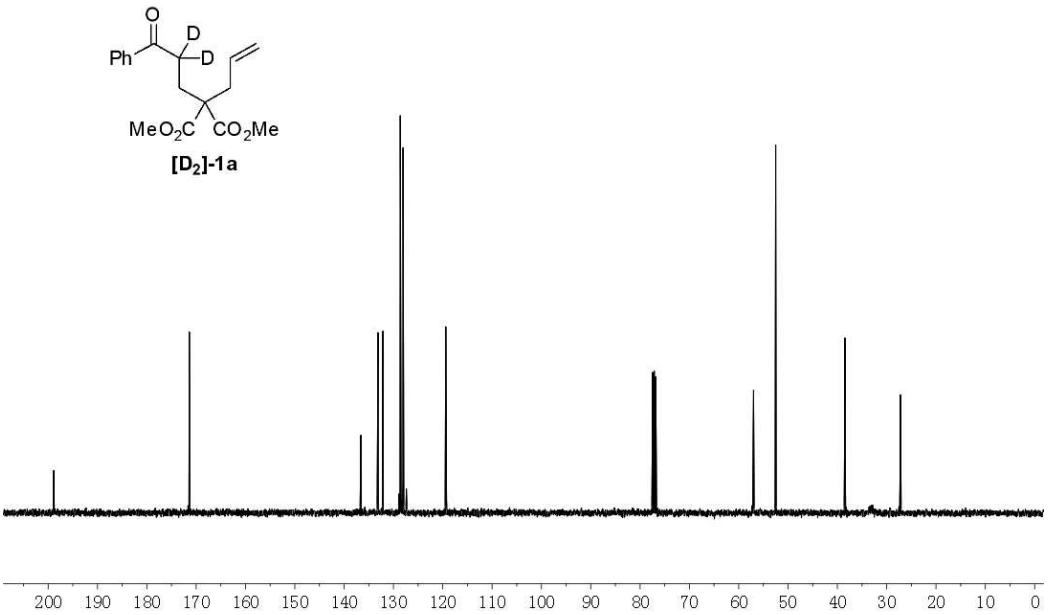
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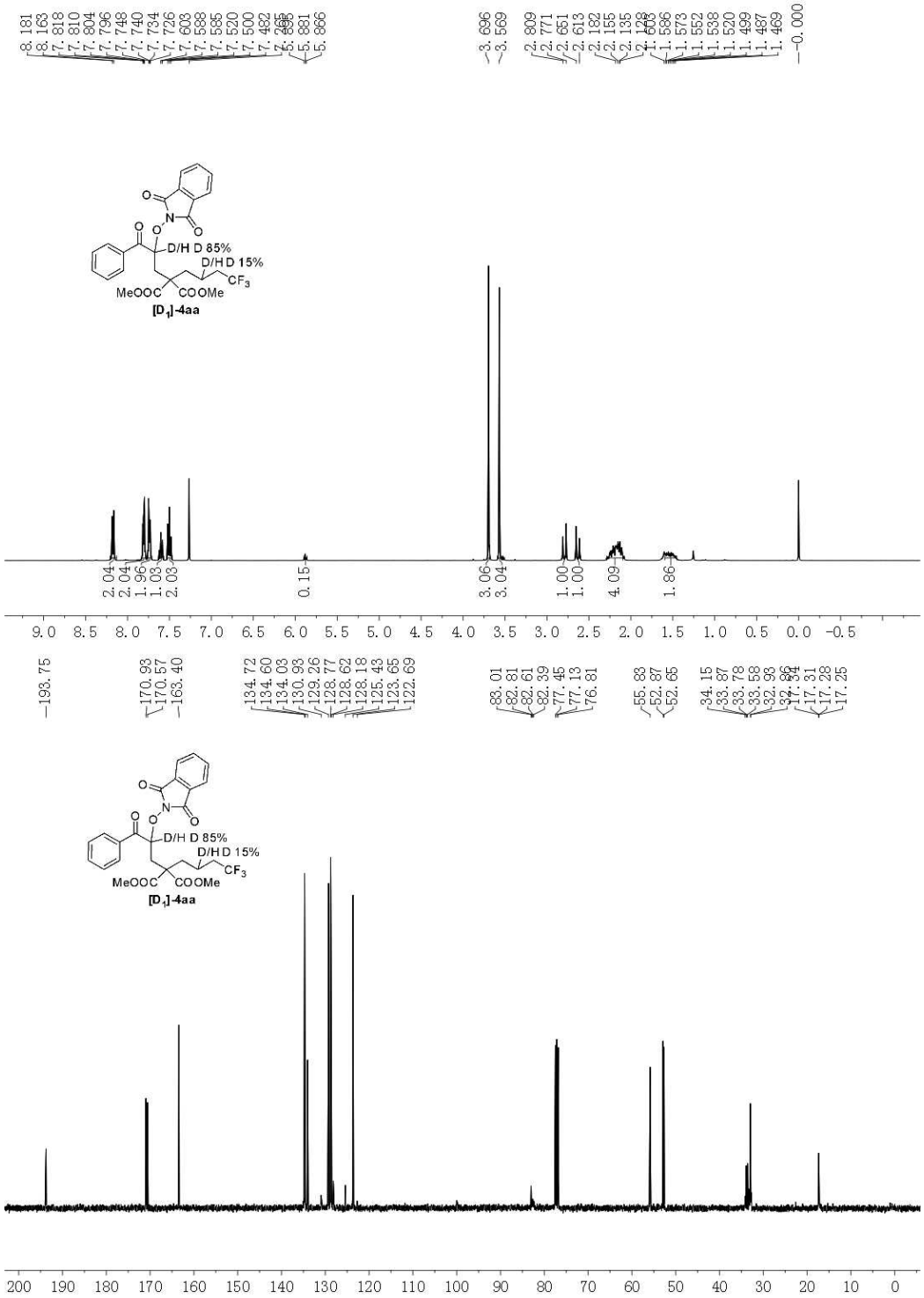
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D/H D 15%
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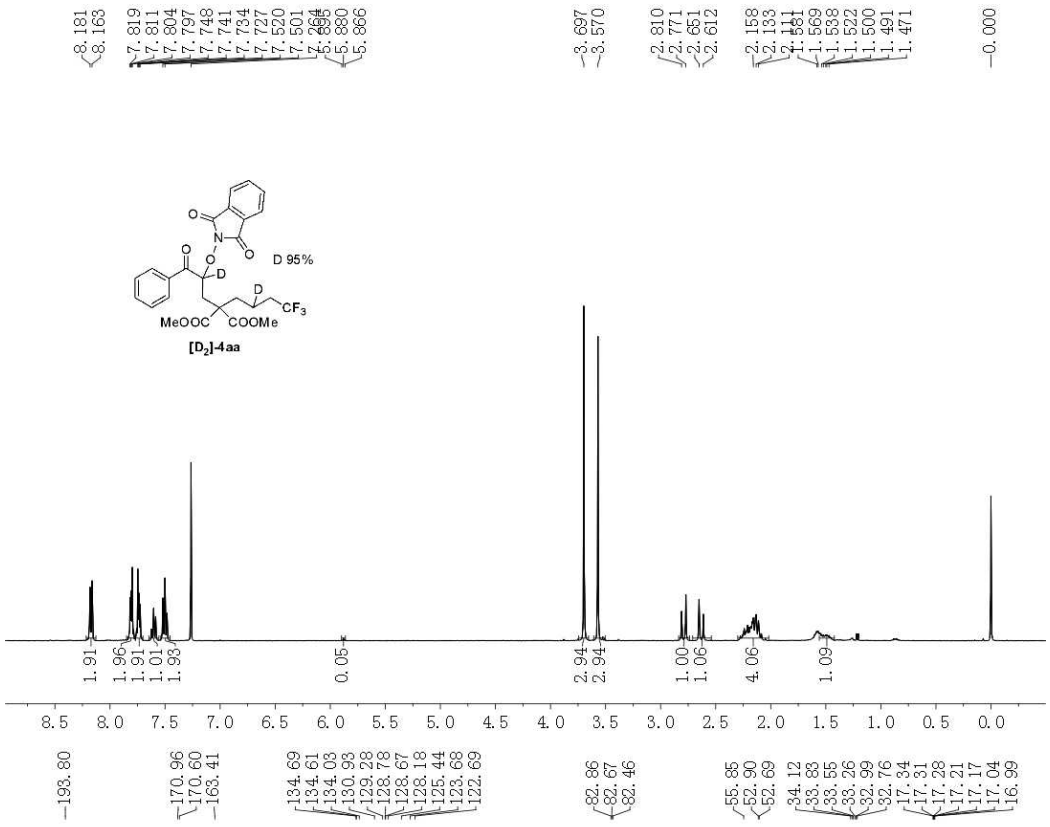
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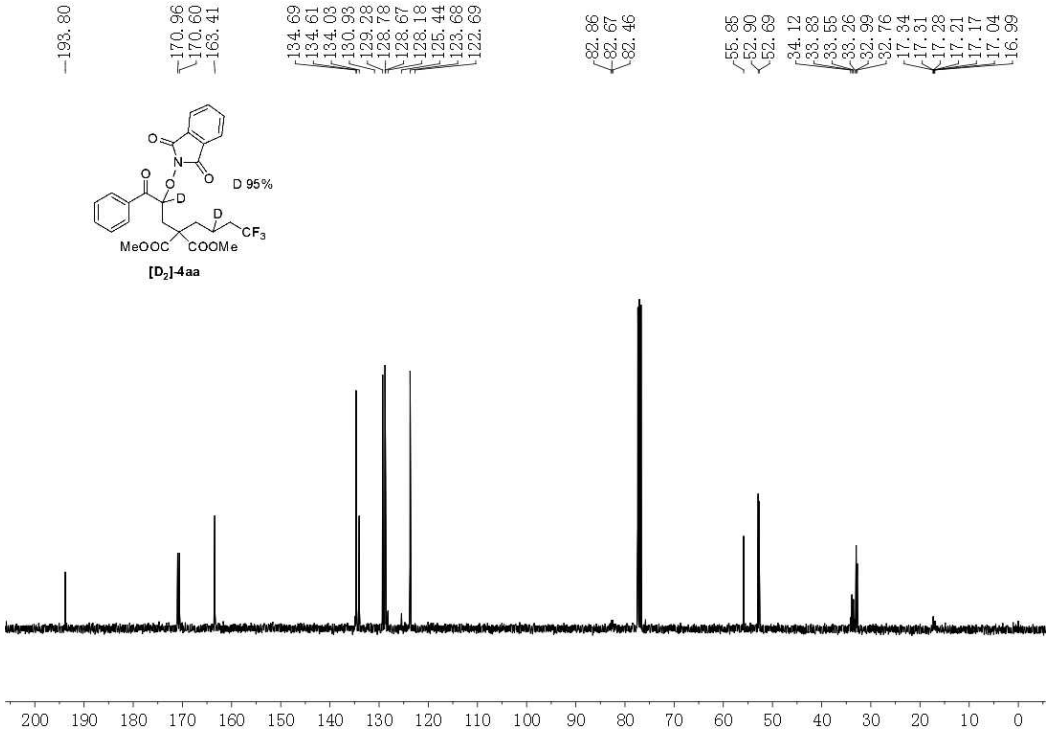
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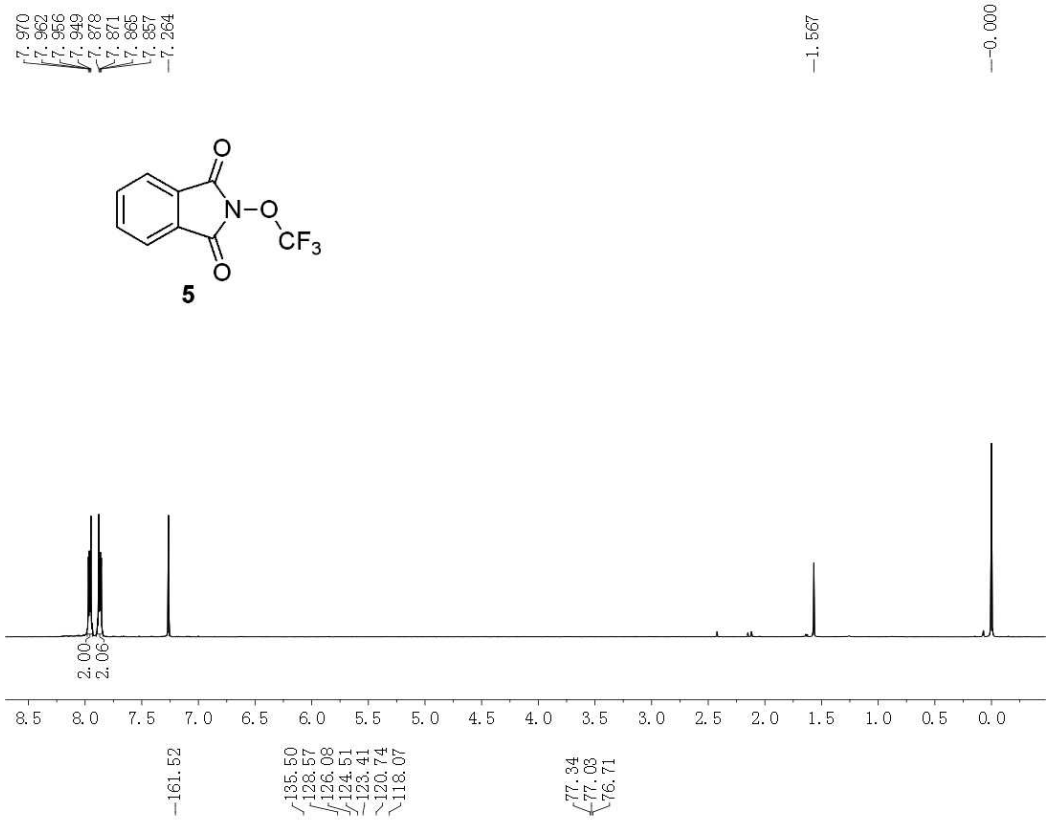
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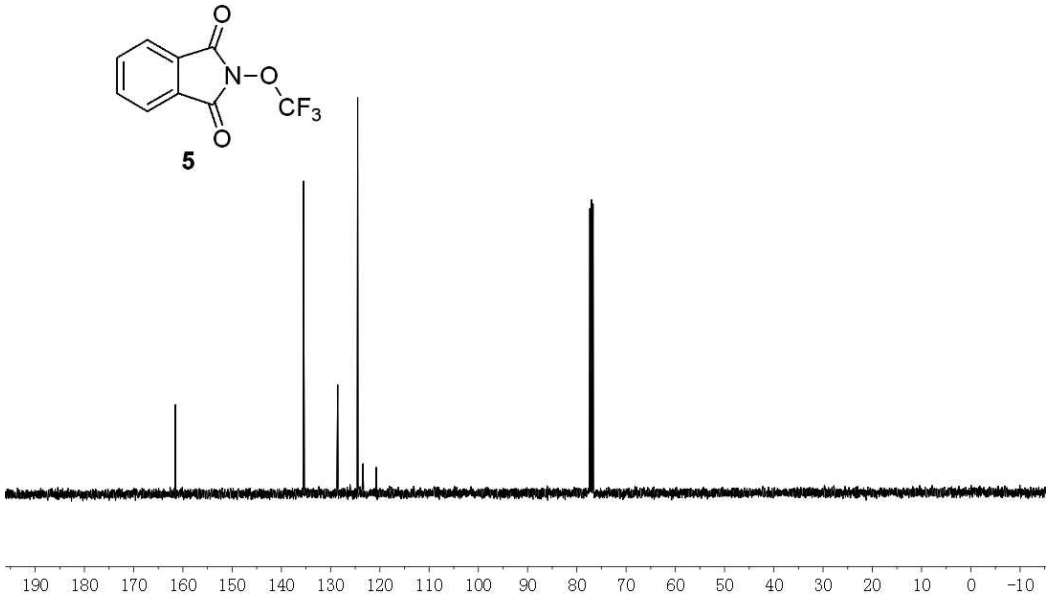
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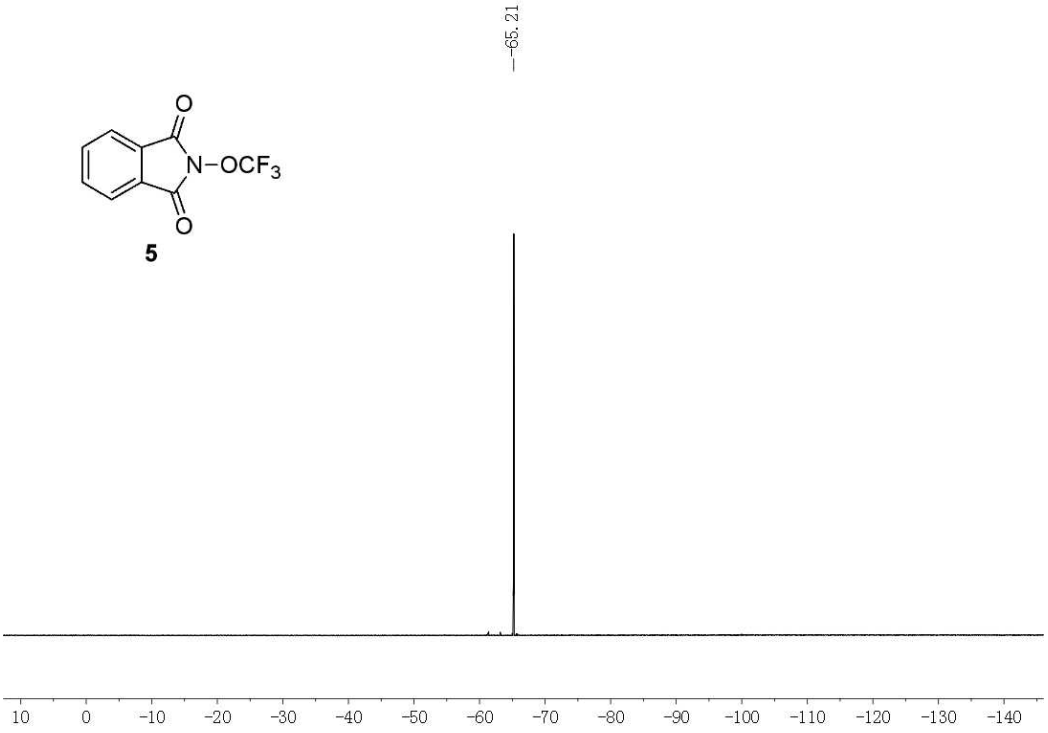
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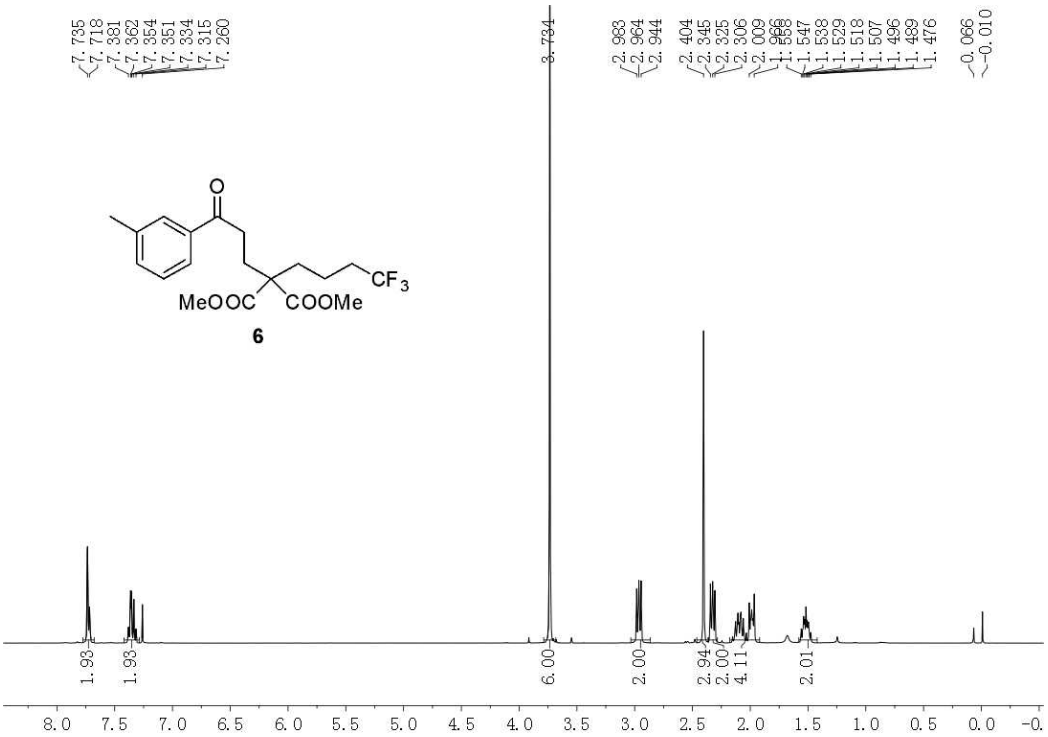
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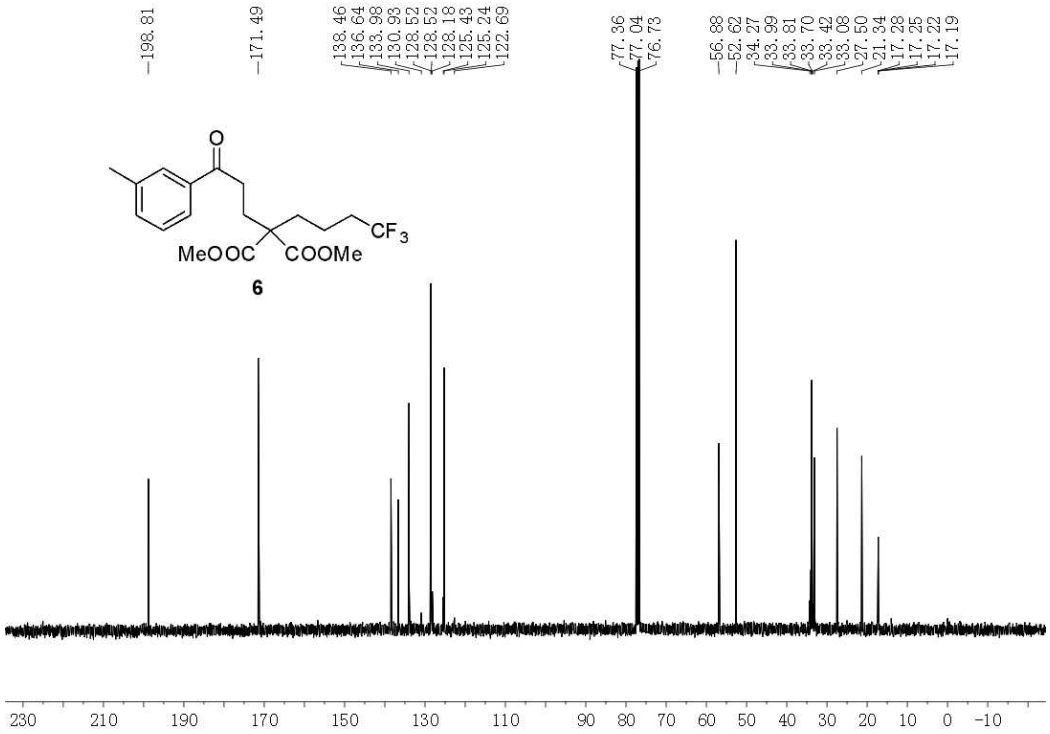
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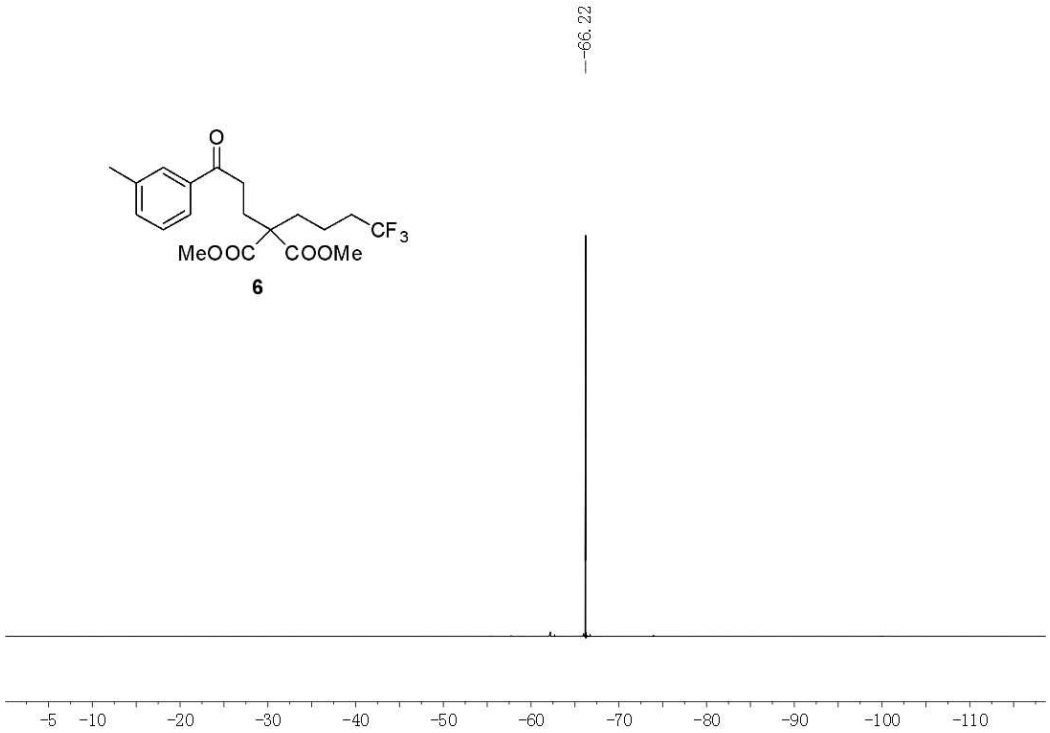
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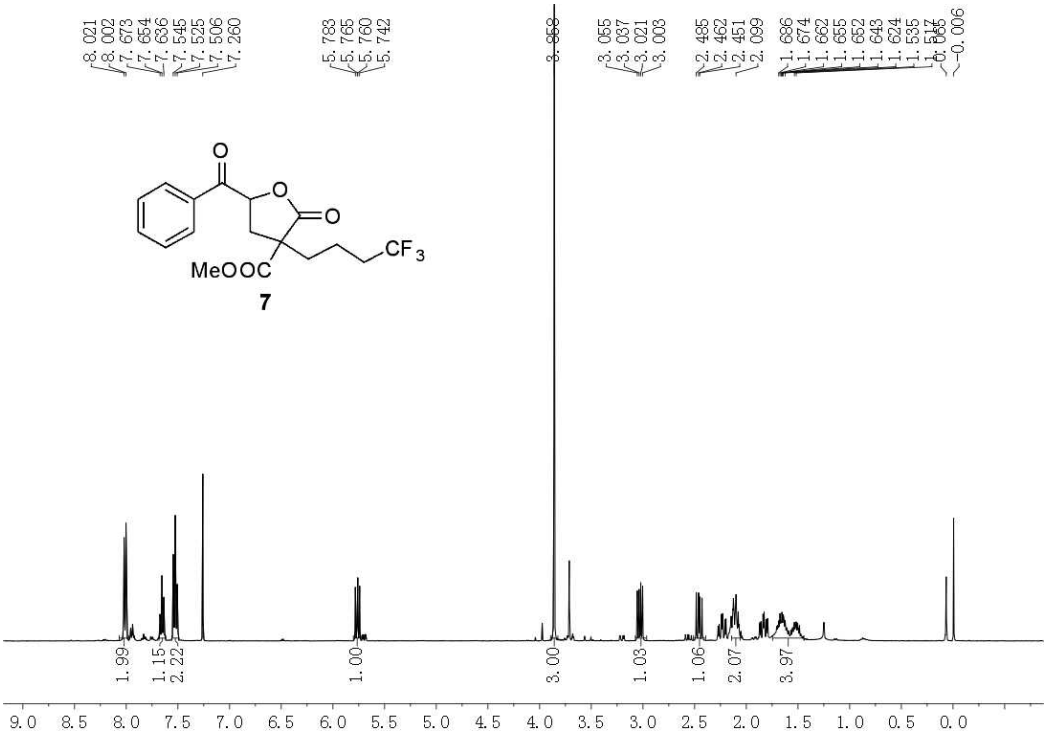
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2.07
3.97
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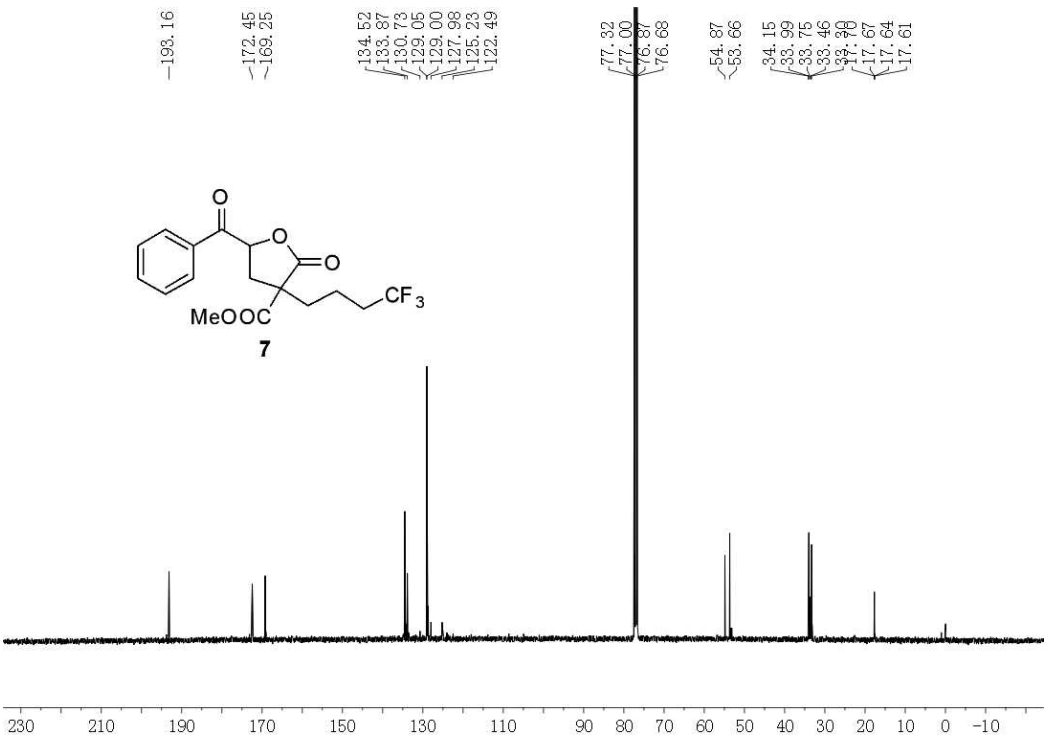
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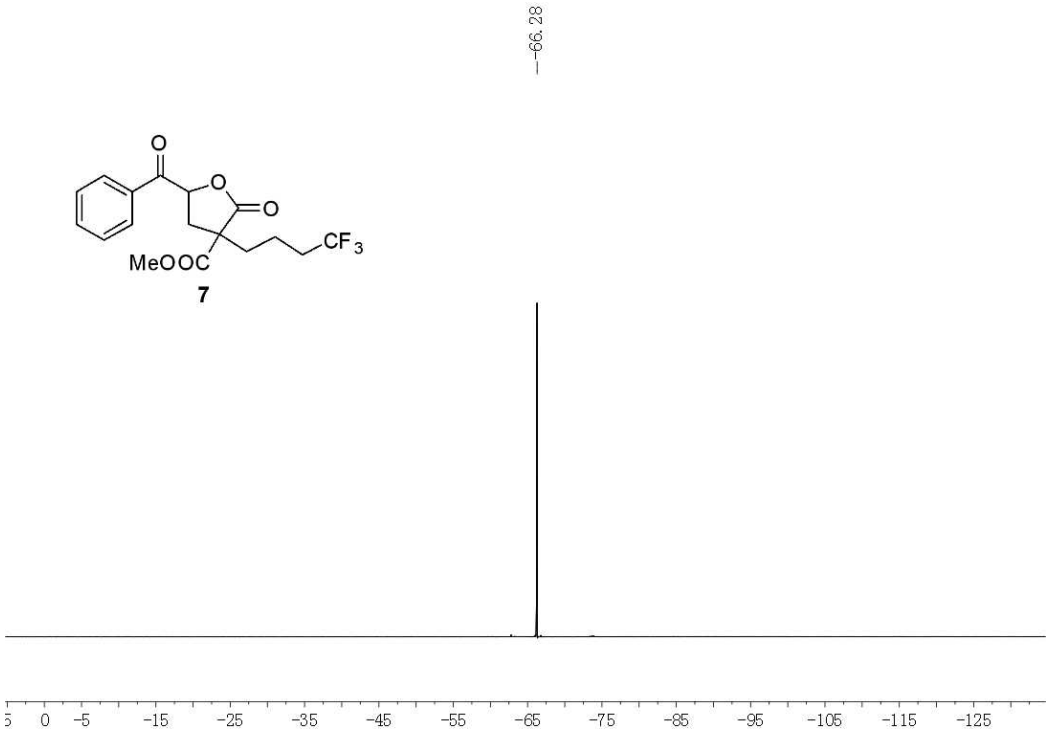
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